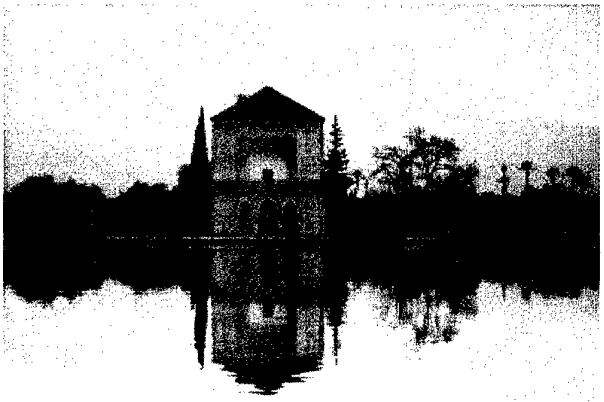
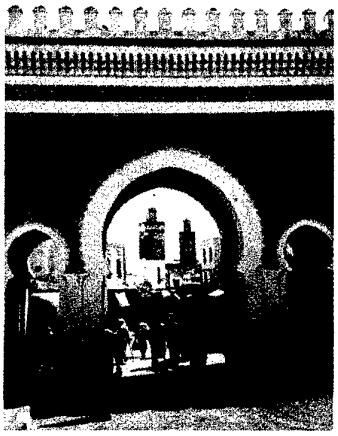
IUTAM

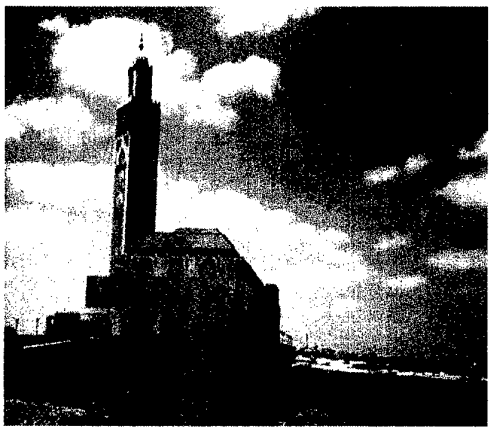
IUTAM Symposium on Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials

October 20-25, 2002

Marrakech, Morocco







Final Program and Abstracts

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IUTAM Symposium on Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials, held 20-25 October 2002 in Marrakech, Morocco. It includes the symposium program and 62 abstracts (total of 80 pages) plus a two page assessment of the symposium by A.S. Argon..

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ABSTRACT (Maximum 200 words)

The topics presented were wide ranging and included many aspects of deformation and fracture in a variety of materials. Among the areas that were considered were:

- Developments on the constitutive connections for inelastic deformation of crystalline media, using atomistic approaches to processes such as cross slip of dislocations, but more often using dislocation models of plastic flow through formalisms of dislocation dynamics but also using models of collective dislocation activity to model incipient patterning and strain hardening.
- Development of deformation textures in polycrystals.
- Problems involving strain gradient plasticity on the sub-Micron scale.
- Problems involving twinning in crystal plasticity and in the context of shape memory behavior.
- Plasticity of amorphous and semi crystalline polymers.
- Plasticity and fracture-related damage development in heterogeneous materials, granular materials, and composites, including the role of grain boundaries.
- Problems involving fracture and its mechanisms ranging from brittle cleavage to ductile cavitational forms and brittle to ductile fracture transitions, as well as in cyclic deformations.

A large number of other topics related to the general theme were also presented in both the main sessions and in the poster presentations.

14. SUBJECT TERMS

Army, Foreign document, Morocco, Crystal Plasticity, Brittle crystal, Polycrystals, Experiments, Modeling, Bioceramic shell structure, Crystalline Granular materials, Fatigue analysis, Polymers

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IUTAM SYMPOSIUM ON MULTISCALE MODELING AND CHARACTERIZATION OF ELASTIC-INELASTIC BEHAVIOR OF ENGINEERING MATERIALS

Held in Marrakech, Morocco
October 20-25, 2002

(An Assessment of the Symposium)
by

A.S. Argon
Massachusetts Institute of Technology
Cambridge, MA 02139 USA

The effective modeling of the often complex properties and mechanical behavior of engineering materials very often requires an approach over a wide range of scales starting from the atomic scale of nanometers to microstructures on the micron scale to finally the technological macroscopic scale. The purpose of the symposium was to address these issues in a variety of contexts.

The symposium was organized in 7 half-day sessions over a period of 4 days. There were 52 presentations including 4 plenary lectures. There were also 2 poster sessions with 12 total posters being presented with 5-minute introductions for each poster.

The topics presented were wide ranging and included many aspects of deformation and fracture in a variety of materials.

Among the areas that were considered were:

- Developments on the constitutive connections for inelastic deformation of crystalline media, using atomistic approaches to processes such as cross slip of dislocations, but more often using dislocation models of plastic flow through formalisms of dislocation dynamics but also using models of collective dislocation activity to model incipient patterning and strain hardening.
- Development of deformation textures in polycrystals.
- Problems involving strain gradient plasticity on the sub-micron scale.
- Problems involving twinning in crystal plasticity and in the context of shape memory behavior.
- Plasticity of amorphous and semi crystalline polymers.
- Plasticity and fracture-related damage development in heterogeneous materials, granular materials, and composites, including the role of grain boundaries.
- Problems involving fracture and its mechanisms ranging from brittle cleavage to ductile cavitational forms and brittle to ductile fracture transitions, as well as in cyclic deformations.

A large number of other topics related to the general theme were also presented in both the main sessions and in the poster presentations.

A particularly satisfying feature of the symposium was the quite substantial number of experimental studies presented that were often successfully integrated into models at the appropriate scale of the phenomena. The discussions of the presented material were often vigorous but good-natured.

The breaks between blocks of lectures and the several planned excursions were also well arranged and reinforced the effectiveness of exchange of ideas and fostered camaraderie. The overall atmosphere at the symposium site in the Imperial Borj Hotel was excellent.

The symposium functioned smoothly and was quite successful in fostering exchange of ideas, information and for the establishment of potentially useful professional contacts between participants. For all these positive aspects credit goes to organizers and to the IUTAM organization for having made a successful selection.

Sponsors

- International Union of Theoretical and Applied Mechanics
- Moroccan State Secretary for Scientific Research
- Pacific Northwest National Laboratory, WA, USA
- European Research Office of the US Army
- University Cadi Ayyad, FSSM, Marrakech, Morocco
- University of Metz, UFR MIM, Metz, France

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M. Ben-Salah	(Fac. Sc.- Rabat)

AQ F03-06-1031

Symposium Program

Sunday October 20

16h – 19h Registration at the Hotel Imperial Borj

Monday October 21

7h30 – 8h00 Registration at the Hotel Imperial Borj

8h00 Departure to the Cadi Ayyad University - Faculty of Sciences (FSSM)

Chairperson : H. ZBIB

8h30 – 9h10 Opening

9h10 – 10h00 Plenary Lecture 1 : New Developments in the Brittle-to-Ductile Transitions of Fracture in Intrinsically Brittle Crystals and Polycrystals: Experiments and Modeling
Ali S. Argon

10h00 – 10h25 Coffee break

10h25 – 11h15 Plenary Lecture 2 : Dislocation-based Length-Scale in Crystal Plasticity: Experiments and Modeling
Sia Nemat–Nasser

11h15 – 11h40 What about the yield transformation surface determination (austenite ® martensite) with the measurement of austenite and martensite lattice parameters for some shape memory alloys ?
P. Blanc, C. Lexcellent, C. Bouvet and A. Vivet

11h40 – 12h05 Well-Assembled and Crossed-Lamellar Microstructure and Robust Mechanical Properties of Bioceramic Shell Structure
T. Watanabe, K. Kido and S. Tsurekawa

12h10 Departure to the Hotel - Lunch **(Next sessions are held at the hotel)**

Chairperson : K. NEALE

14h00 – 14h25 Application of a variational self-consistent procedure to the prediction of deformation textures in polycrystals
P. Gilormini, Y. Liu and P. Ponte Castañeda

14h25 – 14h50 Characterization of Micro- to Macroscopic Deformation Behavior of Amorphous and Crystalline Polymer
Y. Tomita and M. Uchida

14h50 – 15h15 Cross slip viewed at the nono and micrometer scale
T. Leffers and O.B. Pedersen

15h15 – 15h40 A multiscale micromechanics approach to describe environment effects on crack tip damage under cyclic loading
E.P. Busso, G. Cailletaud, S. Quilici

15h40 – 16h00 Coffee break

16h00 – 16h25 Atomic-scale modelling of the dynamics of dislocation behaviour under stress
D. Bacon and Yu.N. Osetsky

16h25 – 16h50 Coalescence and Evolution of Nanoscale Islands into Polycrystalline Thin Films
M. O. Bloomfield, Y.-H. Im, D.Datta, M.S Shepherd, T.S. Cale

16h50 – 17h15 On the Propagative Plastic Instabilities in Aluminum Alloys
D. Thévenet, M. Abbadi, P. Hähner and A. Zeghloul

17h15 – 17h45 Poster presentations : 5 minutes per person

Effect of some parameters on the elastoplastic behavoir of green sand
R. Ami Saada
Experimental investigation of size effects in thin copper foils
G. Simons, Ch. Weipert, J. Dual and J. Villain
Size effects in thin films : a discrete dislocation study
L.Nicola, E. Van der Giessen and A. Needleman
Characterization of the mechanical behavior of materials using a digital image correlation method
S.M'Guil, C. Husson and S. Ahzi
Shear band spacing analysis in the case of HY-100 steel and TI-6Al-4V alloy
O. Oussouaddi, L. Daridon,S. Ahzi and A. Zeghloul
A differential scheme for the effective moduli of viscoplastic composites
F. El Houdaigui, A. Molinari and L. S. Toth

19h00 **Reception at the Hotel Imperial Borj**

Tuesday October 22

Chairperson : M. KHALEEL

8h15 – 9h05 Plenary Lecture 3 :The non-linear inclusion problem with applications to averaging schemes
Alain Molinari

9h05 – 9h30 Collective Dislocation Behavior in Single Crystalline Aluminum under Indentation
Y. Shitbutani, A. Koyama and T. Tsuru

9h30 – 9h55 Simulation of Powder Processing – Models and Applications for the Ceramics and Powder Metal Industry
H. Riedel

9h55-10h20 Fatigue analysis of structures by multiscale approach
K. Dang Van

10h20 – 10h40 Coffee break

10h40-11h05 Multiscale modelling of localization in sheet metals
K.W. Neale, K. Inal and P.D. Wu

11h05– 11h30 Multiaxial plastic fatigue behavior with multiscale Modeling
A. Abdul-latif, K. Saanouni and J. Ph. Dingli

11h30-11h55 A model for damage opening and sliding of grain boundaries
G. Cailletaud, O. Diard, A. Musienko

11h55-12h20 Gradients of Hardening in Nonlocal Dislocation Based Plasticity
G. Voyiadjis, R. J. Dorgan and R. Abu Al-Rub

Lunch and posters

Chairperson : E. BUSSO

14h00 – 14h25 Global and Local Constraints in the Theory of Compaction of Granular Materials
A.H.W. Ngan

14h25 – 14h50 Three-Dimensional Structures of the Geometrically Necessary Dislocations Generated from Non-Uniformities in Metal Microstructures
T. Ohashi

14h50 – 15h15 Simulation of Texture Evolution in Equal Channel Angular Extrusion of Copper Using a New Flow Field
L.S. Toth, R. Massion, S.C. Baik

15h15 – 15h40 Energy Dissipation Mechanisms in Ductile Fracture
J.W. Kysar

15h40 – 16h00
Coffee break

16h00 – 16h25 Constitutive modeling of viscoelestic unloading of glassy polymers
Y. Remond

16h25 – 16h50 A Microcracking and Spall Based Model to Describe the Dynamic Response of for Brittle Materials under Shock and Penetration Loading
A.M. Rajendran

16h50 – 17h15 On the constitutive theories of power-law materials containing voids
C. Y. Hsu, B.J. Lee and M. E. Mear

17h15 – 17h40 Objective quatification of the ductility within the coupling elasticity-damage behavior : formulation
H. Bouabid, S. Charif -d'ouazzane, Mel Kortbi and O. Fassi-Fehri

17h40 – 18h10 Poster presentations : 5 minutes per person

A new model for dilational plasticity and applications to ductile solids
A.A. Benzerga
Influence of temperature and loading on the characteristics of PLC bands in an Al-Mg alloy
M. Abbadi, P. Hähner and A. Zeghloul
Planar impact simulation for ductile metals
L. Campagne, L. Daridon and S. Ahzi
Validation of the tangent approach for the solution of the non-linear Eshelby inclusion problem
A. Molinari, F. El Houdaigui and L. S. Toth
On plasticity and damage evolution during sheet metal blanking
C. Husson, C. Poizat, N Bahlouli, S. Ahzi, L. Merle and T. Courtin
Thermo-electro-elastic effective proprties of piezoelectric composite materials
N. Fakri and L. Azrar

Wednesday October 23

Chairperson : M. CHERKAOUI

8h15 – 9h05 Plenary lecture 4 : Size Effect of Fine Structures - Experiments and Theory
Pin Tong

9h05 – 9h30 Influence of microstructural parameters on shape memory alloys behavior
E. Patoor, C. Niclaeys, T. Ben Zineb

9h30 – 9h55 Analysis of Ridging in Ferritic Stainless Steels Using Crystal Plasticity Finite Element Method
H. Shin, J.K. An and D.N Lee

9h55-10h20 Grain-Boundary Effects and Ductile Failure Evolution in Crystalline Aggregates
M.A. Zikry and W.M. Ashmawi

10h20 – 10h40 Coffee break

10h40-11h05 Particles cluster effect on the damage and failure of metal-matrix composites : micromechanical approach
K. Derrien and D. Batiste

11h05– 11h30 A chesive segments approach for crack growth
J.J.C. Remmers, R. de Borst and A. Needleman

11h30-11h55 Atomistic simulations of materials deformation at high-strain rate
J.A. Young, E.M. Bringa and B.D. Wirth

11h55-12h20 Homogenization techniques based on statistical continuum appraoches
H. Garmestani, B. L. Adams, G. Salehi

Lunch and posters

Marrakech Tour (Departure at 14h)

Thursday October 24

Chairperson : H. GARMESTANI

8h15 – 8h40	Microstructure design for polycrystallne metrerials **B.L. Adams, M. Lyon, S. R. Kalidindi and H. Garmestani**
8h40– 9h05	Reaction-Diffusion Approach to Self-Assembled Nanostructure Formation in Thin Films **D. Walgraef**
9h05 – 9h30	Multi-axial Behavior of Polycrystalline Shape Memory Alloy and Its Constitutive Equations **M. Tokuda, M. Ye, T. Inaba, B. Bundara and P. Sittner**
9h30 – 9h55	Mesoscopic simulations of easy-glide and stage II hardening **A.A. Benzerga, A. Needleman, Y. Bréchet and E. Van der Giessen**
9h55-10h20	Prediction of Damage in Randomly Oriented Short Fiber Composites by Means of A Continuum Damage Mechanics Approach **B. N. Nguyen and M.A. Khaleel**
10h20 – 10h40	Coffee break
10h40-11h05	Non-steady plane strain ideal plasic flow considering elastic dead zone **K. Chung and W. Lee**
11h05– 11h30	Role of deformation twinning in mechanical response of FCC and HCP metals **S.R. Kalidindi, A. Salem and R.D. Doherty**
11h30-11h55	Multiscale Modelling of Non-linear Behaviour of Heterogeneous Materials: Comparison of recent homogenisation methods **P. Kanoute and J.L. Chaboche**
11h55-12h20	Thermomechanical behaviour of shape memory alloy **M.O. Ben-Salah, L. Boulmane and A. Hihi**
	Lunch and posters

Chairperson : S. AHZI

14h00 – 14h25	Multiscale Dislocation Dynamics Plasticity **H. Zbib**
14h25 – 14h50	Prediction of mechanical properties and damage evolution in polymeric composites through meso-mechanical modelling **F. Ellyin, Z. Xia and Y. Zhang**
14h50 – 15h15	Response of TI-6AI-4V alloys over a wide range of strain rates and temperatures and constitutive modelling **A.S. Khan**
15h15 – 15h40	A stress-strain mixture law without fitting parameter application to several classical problems of heterogeneous material behaviour **O. Bouaziz and P. Buessler**
15h40 – 16h00	Coffee break
16h00 – 16h25	On anisotropic formulations of multiplicative inelasticity **C. Sansour**
16h25 – 16h50	Deep drawing process of an AISI304 stainless steel : interaction between geometry tools and kinetics of plastic induced martensite from a micromechanical framework. **Z. Tourki and M.Cherkaoui**
16h50 – 17h15	Modelling and simulation of dynamic plasticity and failure in ductile metals **L. Daridon, L. Campagne, C. Poizat and S. Ahzi**
17h15 – 17h40	Effects of polymeric additives on the morphology and the structure of the calcium carbonate material **A. Jada**
17h40 – 18h	**Closing Remarks**

19h **BANQUET: Departure from the hotel at 19h**

Friday October 25

All Day Tour: City of Essaouira (Departure 07h15 - Return 19h00)

ABSTRACTS

IUTAM Symposium on "Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials" in Marrakech – Morocco, October 20-25, 2002

New Developments in the Brittle-to-Ductile Transitions of Fracture in Intrinsically Brittle Crystals and Polycrystals: Experiments and Modeling

A. S. Argon
Massachusetts Institute of Technology,
Cambridge, MA 02139, U.S.A.

The transition of fracture in intrinsically brittle crystalline solids between brittle and ductile forms of behavior, and vice-versa, have been of concern for a long time from both mechanistic considerations on the atomic level as well as from phenomenological considerations on the macroscopic level. While much progress has been made in recent times, much controversy still remains on how to explain some basic phenomena.

In this lecture we briefly review some recent experimental results and associated crack-tip dislocation models of brittle-to-ductile transition of cleavage fracture in *Si* and *Fe-3%Si* alloy single crystals by a crack arrest method. We then present new experimental results and related detailed models of the effect of high-angle grain boundaries on the cleavage crack propagation resistance of polycrystals of *Fe-3%Si* alloy. The results indicate a three-fold increase of cleavage cracking resistance due to grain boundaries over that of single crystals, with nearly no important grain size dependence.

IUTAM Symposium on "Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials" in Marrakech – Morocco, October 20-25, 2002

Dislocation-based Length-Scale in Crystal Plasticity: Experiments and Modeling

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Plastic deformation of a broad class of metals occurs by the motion of dislocations. The structure of dislocations, their density and distribution, as well as their interaction with each other and with the solute atoms and other defects lie at the foundation of crystal plasticity. Collectively, all these affect the motion of dislocations and, hence, the resulting plastic flow. The collective resistance to the dislocation motion defines the flow stress of the material at the continuum scale. Based on the results of systematic experiments on numerous commercially pure metals, the rate- and temperature-dependence of the flow-stress has been modeled by the author. This modeling naturally involves length-scales that characterize the underpinning dislocation activities. The introduction of the density of dislocations and its evolution, into the constitutive relations appears to be sufficient to account for essentially all existing experimental results that otherwise cannot be modeled by the classical plasticity theories. Rate- and temperature-dependence of the material response are accounted for as an integral part of the kinematics and kinetics of the dislocation motion. The general approach applies to both single crystals and polycrystals. With slight modification, it also applies to the phenomenon of dynamic strain-aging (at high and low strain rates) that stems from the interaction between dislocations and solute atoms.

References:

Nemat-Nasser, S. and J. Isaacs, "Direct Measurement of Isothermal Flow Stress of Metals at Elevated Temperatures and High Strain Rates with Application to Ta and Ta-W Alloys," *Acta Materialia*, Vol. 45, No.3 (1997), 907-919.

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Cheng, J., S. Nemat-Nasser, and W. Guo, "A Unified Constitutive Model for Strain-rate and Temperature Dependent Behavior of Molybdenum," *Mechanics of Materials*, Vol. 33 (2001) 603-616.

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IUTAM Symposium on "Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials" in Marrakech – Morocco, October 20-25, 2002

Application of a variational self-consistent procedure to the prediction of deformation textures in polycrystals

Pierre Gilormini[1], Y. Liu[2] and P. Ponte Castañeda[2]
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A fundamental problem in mechanics of materials is the computation of the macroscopic response of polycrystalline aggregates from the properties of their constituent single-crystal grains and the microstructure. In this paper, the non-linear homogenization method of deBotton and Ponte Castañeda [1] is used to compute "variational" self-consistent estimates for the effective behavior of various types of polycrystals. In contrast with earlier estimates of the self-consistent type, such as those arising from "incremental" and "tangent" schemes, the new estimates are found to satisfy all known bounds, even in the strongly nonlinear, rate-insensitive limit. Earlier papers [2] have detailed the possibilities and the "instantaneous" mechanical response given by the variational self-consistent estimate for various polycrystals, but the present study focuses on the evolution the crystallographic texture predicted by this procedure.
The homogenization scheme allows the characterization [3] of the evolution of the microstructure in a self-consistent fashion by making use of appropriate estimates for the average strain-rate and vorticity within the grains. The complete scheme will be describe and used to model some simple deformation processes, and the results will be compared with available experimental results and with the predictions of other schemes.

References:

[1] G. deBotton and P. Ponte Castañeda. "Variational estimates for the creep behavior of polycrystals." *Proceedings of the Royal Society of London* A **448** (1995): 121-142
[2] M. Nebozhyn, P. Gilormini and P. Ponte Castañeda. "Variational self-consistent estimates for cubic viscoplastic polycrystals: The effects of grain anisotropy and shape." *Journal of the Mechanics and Physics of Solids* **49** (2001): 313-340
[3] P. Ponte Castañeda. "Nonlinear polycrystals with crystallographic and morphological texture evolution." *In Continuum Models and Discrete Systems* (CMDS 9), edited by E. Inan and K. Z. Markov, 228-235. Singapore: World Scientific, 1998.

IUTAM Symposium on "Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials" in Marrakech – Morocco, October 20-25, 2002

Well-Assembled and Crossed-Lamellar Microstructure and Robust Mechanical Properties of Bioceramic Shell Structure

Tadao WATANABE, Kota KIDO and Sadahiro TSUREKAWA
Laboratory of Materials Design and Interface Engineering
Department of Machine Intelligence and Systems Engineering
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The potential and importance of ceramics have been increasingly recognized as structural materials and functional materials. It is our general recognition that ceramics are very much harder and much more brittle than metallic materials. However, there are many living creatures which are partly composed of ceramics: for example shells are composed of aragonicte $CaCO_3$, and animal bones of hydroxyapatite. It is interesting to study how 'intrinsically brittle' ceramics are organized and assembled to be used as components in natural living structures to meet specific requirements for their desirable function and performance.

This paper reports several important findings based on SEM observations of microstructures in a shell (Japanese hard clam) which is popular and called by academic name "Meretrix Lusoria", and "Hamaguri" in Japanese. Several samples were cut out from different parts of a clam and the cross sectional area of the shell as observed and then mechanical tests (hardness test) were carried out to measure the hardness and fracture toughness. It was found that several macro-layered structures and micro crossed-lamellar structure in each layer existed. In the middle region of the cross sectional surface, network aragonite structures were observed on the both side of the central line which is characterized by linking holes. The observed values of Vickers hardness which were determined by indentation perpendicular to the clam surface, ranged from about 100 to 1440, depending on the range of load (0.1~1kgf). The fracture toughness determined from the crack length measured by SEM observations ranged from 0.6MPam$^{1/2}$ to 2.86MPam$^{1/2}$.

The highest observed value of the fracture toughness corresponds to the almost top value for common rocks. The origin of such high fracture toughness will be discussed in connection with the occurrence of micro crossed-lamellar structure.

IUTAM Symposium on "Multiscale Modeling and Characterization of Elastic-Inelastic Behavior of Engineering Materials" in Marrakech – Morocco, October 20-25, 2002

What about the yield transformation surface determination (austenite → martensite) with the measurement of austenite and martensite lattice parameters for some shape memory alloys ?

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If one choose the n lattice correspondant variants (l c v) as internal variables for the martensitic phase (n = 12 for monoclinic martensite), with the values of lattice parameters of Austenite (A) and Martensite (M) cells, the phase transformation (P.T.) strain tensor $\underline{E}^{tr}$ can be determined. Moreover, the yield surface for phase transformation (A → M) can be obtained. An homogeneisation process permit to predict the shape of the P.T. surface for polycrystals under multiaxial proportional loading. A comparison with on one side a prediction of a phenomenological model at the macroscopic scale and an another side with the experimental points obtained under biaxial loading is fairly good for Cu Al Zn, Cu Al Be or Ni Ti alloys. One has to note that the classical assymmetry between tension and compression is taken into account.

If one choose the habit plane variant (h p v) as internal variables, the situation is the same for Cu-based alloys because it exist an "exact" interface between austenite and only one variant of martensite, it means that h p v are l c v. But for Ni Ti, one has to examine two compatibility conditions : (i) one between i and j variants, (ii) the other between (i,j) and the mother phase A (number of h p v for Ni Ti : 192).

After an homogeneisation process, the prediction of yield P.T. surface for polycrystal Ni Ti is a little surprizing, because the assymmetry between tension and compression (classicaly experimentally observed) is not predicted.

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Characterization of Micro- to Macroscopic Deformation Behavior of Amorphous and Crystalline Polymer

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The purpose of the present study is to elucidate the micro- to macroscopic deformation behavior of an amorphous and crystalline polymer. The distribution of the number of entanglement points of molecular chains is introduced, and the micro- to macroscopic deformation behavior is investigated by means of computational simulation with the nonaffine molecular chain network model. The results clarified the onset of microscopic shear bands emanating from the slightly weak points and their evolution and unification to the macroscopic shear band. The characteristic feature of deformations for macroscopically uniform tension, compression and shearing, and the evolution of surface undulation under compression have been demonstrated. With regard to the crystalline polymer containing amorphous phase, suitable model accounting for the interface effects with characteristic length scale is presented and their macroscopic manifestations are explored.

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CROSS SLIP VIEWED AT THE NANO- AND MICROMETER SCALE

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The results of recent work on atomic-scale modelling of cross slip of non-jogged and jogged screw dislocations are summarized – with special emphasis on the activation energy for cross slip. The results are compared with microstructural observations on cyclically deformed copper and with observations on the texture transition in brass. The indication is that cross slip plays a governing role in cyclic deformation/fatigue and in texture formation.

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A Multiscale Micromechanics Approach to Describe Environmental Effects on Crack Tip Damage Under Cyclic Loading

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A large proportion of the service life of high temperature single crystal components is taken up in initiating and growing fatigue-induced surface cracks. The dominant mechanism of fatigue crack growth in single crystal superalloys is known to be the linking up of microcracks which nucleate at pre-existing 10 to 20 μm casting-related porosities. Furthermore, the crack growth behaviour is controlled by thermally induced stresses and strongly affected by the local microstructural degradation around the crack faces caused by oxidation and interdiffusion processes.

In this work, a multiscale mechanistic approach is employed to study the effects of environment, microstructure and damage of the local crack tip stress and strain fields. At the macroscale (i.e. component level), the effect of a reduction in the volume fraction of the γ' precipitate phase in Ni-base superalloys on the time-dependent crack tip stresses is analysed numerically. Such variations can be related to the microstructural degradation caused by oxidation and diffusion processes. The approach relies on a recently proposed multi-scale rate-dependent crystallo-graphic theory to describe the macroscopic constitutive behaviour of the single crystal in terms of material parameters which depend explicitly on the characteristics of the precipitate phase at the microscale.

At the mesoscale (i.e. porosities), a micromechanics-based formulation is relied upon to describe the initiation of fatigue cracks from initially spherical defects. The effects of stress state, temperature and interaction with a free surface on the local stress variations within a loading cycle are quantified from detailed finite element analyses of a representative material volume containing a void. Based on these results, as a meso-mechanics Weibull-type formulation for fatigue crack initiation is presented and implemented within the finite element method.

Coupled diffusion-damage-stress finite element analyses on a typical compact tension specimen are conducted to quantify the dependency of the local crack tip stresses and strains on the locally degraded precipitate population and on porosity-related damage. The implications of these findings in relation to the microstructural degradation caused by oxidation at cracks faces are discussed

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Atomic-scale modelling of the dynamics of dislocation behaviour under stress

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Reliable application of continuum-based dislocation dynamics models of plasticity require as input detailed information on the way dislocations respond to stress at the atomic level. An obvious example of such information is the relationship between dislocation velocity and temperature, applied stress, dislocation character and crystal structure. Another is the resistance and configuration changes dislocations experience due to obstacles to their glide in the microstructure. As part of a programme to apply multiscale modelling techniques to study plasticity in metals subjected to radiation damage, we have extended the model of Baskes and Daw [1] to use molecular dynamics and statics to investigate the behaviour of dislocations at the atomic level. The method has been applied initially to edge dislocations in □-iron moving over large distances on the atomic scale under various conditions of applied shear stress (with constant or variable strain rate) and temperature. The model will be discussed in terms of the sensitivity of stress-strain curves and 'Peierls' energy barriers to model size and other parameters. Results will also be presented from investigations of dislocation pinning effects and passing mechanisms for radiation-induced obstacles such as voids and secondary phase coherent precipitates of copper.

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Coalescence and Evolution of Nanoscale Islands into Polycrystalline Thin Films

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We show results of physically based simulations of microstructure development during long throw physical vapor deposition (LTPVD) of a thin metallic film on a bare substrate. The simulations show how deposited material first form islands and then coalesce into a blanket film (see Figure 1). In our simulations, the mean free path of atoms in flight is taken to be long compared to the length scale of the grains, and thus the system is in a ballistic transport regime. Transport is solely along line-of-sight paths, and solid-gas collisions dominate over gas phase collisions. Arriving metals atoms have relatively low energy, and sticking factors are taken to be unity.

Due to the long-throw aspect of the system, the particle distribution function (PDF) of the incoming metallic species is regarded as a Gaussian distribution with very narrow width, orientated toward the sources. Shadowing effects of larger, broad grains are accounted for, and the resulting simulation, which does *not* assume a "solid on solid" model, exhibits voiding. The grain boundaries that form as islands impinge upon each other are no longer available for deposition from the LTPVD source, but are allowed to evolve further under curvature driven motion, to minimize grain boundary energies.

A finite element based level set code is used to track the resulting changes in geometry and topology, This method allows us to attach properties, *e.g.,* orientation and composition, to each grain. Another finite element code can be used to track transport and reaction in the fluid phase above the evolving surface for non-ballistic regime systems. These systems can include electrochemical and electroless plating.

This effort extends multiscale process simulation work that integrated reactor-scale and feature-scale simulations [1,2] by allowing inclusion of the grain scale. Information from the reactor scale is passed to the deposition model on the grain scale, and the evolution of the thin film microstructure is tracked. Reactant consumption information is fed back to the intermediate and reactor scale to update these larger scales. We calibrate the process model based upon comparing the predicted grain structures to experimental measurements of actual grain structures.

Figure 1: Nanocrystalline "islands" evolving with time, and coalescing into blanket films. This simulation took 10 minutes, using 1 SPARC IIe processor per grain orientation.

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On the Propagative Plastic Instabilities in Aluminum Alloys

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In crystalline materials plastic deformation is intrinsically heterogeneous at a microscopic scale but continuous at a macroscopic level. However, several cases of heterogeneous plastic flow at a macroscopic scale are known in the literature with their physical origin at the microscopic level. There are two types of frequently observed propagative plastic instabilities associated with nonuniform and unstable flow : the Piobert-Lüders (PL) bands and the Portevin- Le Chatelier (PLC) effect. The PL bands propagate along the axis of a tensile specimen during the early stage of deformation at constant applied load, and after their passage, the material is left in an almost homogeneously strained state (extended yield phenomenon). As opposed to the PL bands, the PLC effect generally initiates after a finite amount of plastic strain and consists in the repeated nucleation and/or propagation of deformation bands. These instabilities appear as the result of the phenomenon of strain ageing which is common in alloys containing solute that segregate strongly to dislocations. Two types of strain ageing can be characterized – static strain ageing where the ageing process takes place after prestraining, and dynamic strain ageing where ageing is sufficiently rapid to occur during straining. The particular point of interest is that both types of strain ageing can also give rise to inhomogeneous plastic deformation. Static strain ageing results in the appearance of the PL strain phenomenon and dynamic strain ageing produces a variety of types of inhomogeneous deformation (the PLC effect) characterized by terms such as "serrated yielding", "jerky flow" or "serrated flow".

Inhomogeneous deformation exerts a detrimental influence in all three areas concerning the mechanical behaviour of materials : testing, structural strength and forming. The testing of mechanical properties is usually performed on tensile specimens or other samples : unless the deformation is uniform, the test data do not represent (local) material properties. In structural applications, it is often important to have a margin of safety if the yield stress should indeed be exceeded : well-controlled plasticity should be preferred to local, unstable behaviour ; and insensitivity to local stress concentration is desirable. In forming applications, there are usually a number of degrees of freedom, both with respect to some components of strain, and with respect to the locations at which straining actually takes place; even if localized deformation does not lead to failure, it may cause disturbing surface irregularities, e. g. in sheet metal forming. Ways to avoid the PL and the PLC regimes have been empirically determined in forming technologies, but the physical mechanisms of localized deformation need to be known in some more detail, with the aim of improving current material properties.

Due to the continuous effort of numerous researchers, there is now a reasonable understanding of the mechanisms and manifestations of the PLC effect. The most salient features of the effect are : serrated stress-strain curves and traces of strain localizations on the specimen surface, easily visible to the naked eye, or by some more sophisticated means. Closer investigation reveals differences in the pattern of stress discontinuities depending primarily on temperature and the rate of deformation. Among the

existing theoretical approaches, we consider a physical model proposed by one of us, the results of which proved to be in close agreement with the experimental results of the present study. The model is based on a physical description of dynamic strain ageing and shows the PLC domain to be delimited at high temperature and loading rate. It also confirms a decreasing trend of band propagation velocity when stress rate increases.

This work is a presentation of experimental data of propagative plastic instabilities for aluminum alloys, with emphasis on the following aspects of the phenomenon :

Strain-rate, stress-rate and temperature dependence of bands characteristics

The critical strain for the onset of serrations

Solute concentration dependence of plastic instabilities

Grain size effect

Effect of ageing

Effect of precipitation

Influence of specimen surface finish on traction curves and bands propagation velocities

Finally, a comparison between some experimentally observed characteristics and those obtained with the mentioned models will be presented.

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EFFECT OF SOME PARAMETERS ON THE ELASTOPLASTIC BEHAVIOR OF GREEN SAND

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The behavior of the casting sands at high temperatures (up to 950 °C) is presented from an experimental viewpoint. Based on a parametric study, the predictions are well discussed and compared with those experimental results. Uniaxial compression tests at different temperatures (20 to 950 °C) and at three strain rate values ($\dot{\varepsilon} = 10^{-2} s^{-1}$, $\dot{\varepsilon} = 10^{-3} s^{-1}$ and $\dot{\varepsilon} = 10^{-4} s^{-1}$) were performed in the foundry sand (Ami Saada et al., 1996, Ami Saada 1997, Ami Saada et al., 1999). They show that casting sands exibit no strain rate effect for the temperatures ranging from 20 to 600 °C. The strength of this material is governed by the presence of bentonite and water : In this case, it may increase or decrease when the bentonite is at the temperature range between (20 to 800 °C) or in the range (800 - 950°C), respectively.
Three elastoplastic models developped by the author (Ami Saada et al., 1996) for the green sand at the temperature range (20 to 600°C), are revisited in this study. Especially, the effect of some parameters on the mechanical behavior of the casting sands are investigated, such as cohesion pressure P_{c0} and the slopes of the swelling and consolidation lines.

Keys words:
Thermal consolidation, Thermoelastoplasticity, Green sand, Core sand, Casting process, Triaxial compression tests, Uniaxial compression tests.

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Experimental Investigations of Size Effects in Thin Copper Foils

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This work deals with the characterisation of the deformation behaviour of thin copper foils with the goal of investigating size effects. Tensile tests are performed with specimens, which possess a constant thickness/width and width/length ratio whereas the thickness varies from 2 to 250 μm. A mandatory requirement for studying size effects is that the specimens tested have a microstructure (e.g. texture, grain size), which is the same for all sample sizes.
The specimens are produced by wet etching out of a foil. The strain measurement for these tiny samples (e.g. cross section of 10 * 200 μm) is performed optically: In the test a CCD camera records continuously images from the specimen, these images are compared to the image of the undeformed specimen, which was acquired at the beginning of the test. Out of this comparison, the strain can be quantified using the LSM (least square template matching) algorithm with a deformation resolution of 20 nm. The force is measured by a balance (resolution 10^{-5} N).

Results show a transition from ductile to "brittle" behaviour in the range of about 20 μm: Foils thinner than 20 μm show hardly any plastic deformation. This fact is interpreted by analysing the fracture surfaces and by establishing a model based on the microstructure.

Further tensile tests with specimens incorporating defects are performed to study the influence of strain gradients. First results are presented.

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Size effects in thin films: a discrete dislocation study

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A discrete dislocation plasticity study is carried out to evaluate the stresses generated in a single crystal coating due to the thermal mismatch with its substrate, and their relaxation by dislocation motion. The problem is modeled in two dimensions assuming plane strain conditions. While cooling from a stress-free configuration proceeds, the stress field is calculated as a superposition of an infinite medium solution for the discrete dislocations and a linear elastic finite element solution to enforce the boundary conditions.
Dislocations in the film are taken to be of edge character only and treated as line singularities in an isotropic linear elastic continuum. A set of constitutive equations governs dislocation generation and glide, and pinning of dislocations at point obstacles.
The simulations track the evolution of the dislocation structure while thermal stress builds up and predict the formation of a hard boundary layer at the interface between film and substrate. This layer thickness does not scale up with the film thickness, hence causing a size effect. Simulations moreover show a reduced nucleation activity in very thin films, which leads to a further increase of their strength.

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CHARACTERIZATION OF THE MECHANICAL BEHAVIOUR OF MATERIALS USING A DIGITAL IMAGE CORRELATION METHOD

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The measurement of displacement fields with accuracy and speed of treatment is important for the experimental work in solids mechanics (characterization of mechanical behavior, metal forming, ...). Several measurement methods exist : classical marking by grids, moiré, holographic technique, speckle, ... All of these methods have limited advantages either in their implementation, range of measurement, accuracy, or speed of treatment.
The proposed non-contact technique allows for a very large strain range measurements and a good accuracy on the measured displacements. This method uses the technique of direct correlation of digital images. It compares directly the pixels of an initial picture with those of an image obtained after distortions of the specimen. The accuracy could reach $1/60^{th}$ of a pixel. Accurate cartography of strain fields can be obtained because more than 15000 measures are conducted. The covered field ranges from few millimeters to few meters. Another advantage of this technique is the abandonment of the classical marking. In fact, a random pattern (speckle type), applied on the surface of specimen using a simple bomb of paint, is sufficient to obtain a measure of displacement fields and distortion fields. The images are taken with a numeric camera. A constant light during the taking of pictures has to be assured. The experimental conditions must be in such a way that any deterioration of the random aspect, deposited on the specimen, will not occur. Lost, alteration or little modification of the speckle aspect will not guarantee the success of the correlation. The mechanical characterization of thin sheet is presented as an example.

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Shear band spacing analysis in the case of HY-100 steel and Ti-6Al-4V alloy

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This work concerns the analysis of the formation of multiple adiabatic shear bands in HY-100 steel and Ti-6Al-4V. We analyze, via analytical criteria and numerical calculations, instability and shear band spacing in simple shear. The Mechanical Threshold Stress (MTS) model [1-3] is used in our proposed analysis. The MTS model is based on the use of the mechanical threshold stress as an internal state variable, which successfully describes the deformation response of metals at high strain rates. We used the perturbation method to analyze the stability of a homogenous solution of the governing equations. In the few existing works in this area, the power [4] and Johnson-Cook [5] laws are widely used and leads to analytical solution [6]. The proposed approach based on the use of the MTS model requires numerical solution for the heat equation and the evolution equation of the internal variable. The shear band spacing is computed using Wright and Ockendon's [7] and Molinari's [8] postulates. The comparison between the two postulates are presented. The effects of loading conditions on the shear band spacing are discussed. The results from the MTS model are compared to those of the Johnson-Cook law and experimental results. In the case of Ti-6Al-4V, the MTS stress model seems to be in a better agreement with the experimental results [9] then that of the Johnson-Cook law and other existing models. We have shown that the MTS model predicts well the value of the shear band spacing, and the influence of strain rate and thermal conductivity on the shear band spacing.

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A differential scheme for the effective moduli of viscoplastic composites

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The differential scheme is used to predict the mechanical behavior of materials constituted of a matrix in which inclusions with different behavior are isotropically dispersed. The different phases have a non linear viscous response. The procedure involves the solution of a non-linear Eshelby inclusion problem. An approximate solution of this problem is provided by the tangent approximation of the matrix behavior as proposed by Molinari et al. (1987-1994).
The proposed differential scheme allows to calculate the effective moduli of the composite, for ellipsoidal inclusions dispersed in the matrix. The construction of the differential method for a two phase viscoplastic composite proceeds as usual. At the first step, an infinitesimal fraction of inclusions is isotropically dispersed in the matrix. For this dilute concentration the interaction between inclusions can be neglected and the local strain rate within each inclusion can be obtained as the solution of a non-linear Eshelby problem (a single ellipsoidal inclusion within an infinite matrix). Then the overall response of this composite material is calculated. This effective medium with new moduli is employed as the base property of the next incremental step, which consists in the dispersion of a new infinitesimal volume fraction of inclusions. The new composite is again homogenized. The procedure is repeated until the right volume fraction of inclusions is obtained.
The effective response of the composite material is calculated as a function of the volume fraction of the spheroids for different values of the relative strength (of inclusions with respect to matrix) and different values of the strain rate sensitivity (identical for both phases).

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The non-linear inclusion problem with applications to averaging schemes

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Eshelby (1957) has solved the inclusion problem in the linear elastic case and for ellipsoidal inclusions. When non-linear behaviors are considered, an approximate solution of the inclusion problem can be obtained by analytical means with a proper linearization of the matrix response, Molinari et al (1987), Molinari and Toth (1994). The non-linear matrix response is linearized by considering a first order Taylor expansion (tangent approach). The overall strain rate is taken as the working point for this Taylor expansion. The resulting solution can be formulated in terms of an interaction law providing the average strain rate in the inclusion as a function of the overall applied strain rate. The structure of this interaction law is similar to the linear case (Eshelby problem) with the tensor of tangent moduli of the matrix playing the role of the tensor of elastic moduli. Note however that the non-linear character of the problem is entirely maintained in the interaction law via the stress-strain non-linear responses of the inclusion and matrix. The interaction law appears as the key result, which provides:

- a non-linear equation for evaluating the average strain rate within the inclusion
- a tool for averaging the mechanical response of non-linear heterogeneous materials

The accuracy of the tangent approach for solving the non-linear Eshelby problem has been evaluated by comparison with Finite Element calculations, Molinari et al (2000). It was shown that the strain rate average within the inclusion was quite well described. However, the strain rate heterogeneity within the inclusion, which is a specific feature of the non-linear Eshelby problem, cannot be analysed with use of the tangent approach. A detailed comparison between the tangent approach and Finite Element calculations is presented by Molinari et al (2002) for various aspect ratios of the ellipsoidal inclusion, different hardness ratios, several loading paths and different strain rate sensitivities.

As for the Eshelby solution in linear elasticity, the tangent approach of the non-linear inclusion problem provides an interesting tool for averaging non-linear responses. First applications are shown for rigid viscoplastic materials sustaining large deformations, Molinari (1997-1999-2002). As for the linear case, averaging schemes are constructed by considering a uniform infinite reference medium. Each phase of the heterogeneous material is represented by a ellipsoidal inclusion embedded in the reference medium. Then, to each phase is associated a non-linear inclusion problem, which has to be solved; this provides an estimation of the average strain rate within each phase in terms of the applied macroscopic strain rate. By a proper choice of the reference medium, different averaging models are obtained (self-consistent scheme, non-linear Mori Tanaka model ...). Due to the fact that no information is obtained on the strain rate heterogeneities within inclusions, the overall response of the aggregate is stiffer than expected. A proper calibration of the interaction law can provide a way to soften the overall response.

When elastic deformations are accounted for, averaging schemes become more difficult to work. However a simple interaction law including elastic effects has been proposed by Molinari et al (1997). This law has been modified and included in a proper averaging scheme, Molinari (2002).

The final part is related to the discussion of averaging methods for materials subjected to very high strain rates. An example is shown where classical averaging schemes fail to predict the right answer. For a porous viscoplastic medium, micro-inertia effects can be significant in the vicinity of pores when high overall strain rates are applied. A composite sphere model has been developed to describe these inertia effects. The Gurson approach is extended to porous viscoplastic materials under dynamic loading, Molinari and Mercier (2001).

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Collective Dislocation Behavior in Single Crystalline Aluminum under Indentation

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A tiny piece involving the indented region is cut from the single crystalline aluminum sample and thinned until a few nanometer thickness by means of the Focus Ion Beam (FIB) technique. Then, the cross sections of the indent-induced plastic zone are observed by the transmission electron microscopy (TEM) in order to know how far the emitted dislocations extend under the indentation stress state and whether or not the internal defect- organization due to the collective dislocations exists. The microhardness drastically increases as the indent depth decreases, as having shown in the some previous references, and the subgrain formation as a result of self-organized patterning of dislocations is recognized at the relatively large indent depth. The molecular dynamics simulations with atoms more than 10**6 are also performed to understand the hardening at the nanometer scale from the viewpoint of generation of the immobile dislocation mechanism.

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Simulation of Powder Processing – Models and Applications for the Ceramics and Powder Metal Industry

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Many materials are processed by powder technological methods. The parts are shaped from the powder by uniaxial die compaction, slip casting or some other shaping process, and are subsequently consolidated by sintering (firing).

Powder technology can benefit from material modelling and numerical simulation in several respects. Established processes with their everyday problems can be improved. For example, the cracking and sinter warpage of ceramic parts can be controlled by simulation-guided tool design and process control. This leads to significant reductions of the development cost and time for new parts. Materials with improved properties and components with new functionalities often require novel production processes, which can be mastered more easily with the aid of realistic simulation tools. The production methods for multilayer electric or electronic components, such as are piezo-actors, solid oxide fuel cells and LTCC's involve many practical problems. Numerical simulation tools for the processing steps tape casting, lamination, drying, binder removal and sintering can help to solve these problems.

Some of the material models used in the simulations are purely phenomenological, while others are based on micromechanical models, such as the models for solid-state and liquid-phase sintering. Some of these models and case studies of industrial problems are described. An attempt is made to identify open questions and new fields within powder technology, where the development of simulation tools appears to be rewarding.

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FATIGUE ANALYSIS OF STRUCTURES BY A MULTISCALE APPROACH

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Current industrial design is concerned with fatigue, as the main failure mode of mechanical structures under variable loadings. The actual prediction techniques use generally fatigue criteria based on stress approaches in the high cycle fatigue (HCF) regime and on strain or inelastic strain approaches in the low cycle (LCF) domain. However, success was obtained when the stress and the strain cycle was uniaxial and simple. This is not always the case, as stresses and strains are often multiaxial and present a complex path during the loading cycle. Application of classical fatigue models to mechanical structures is then difficult and the predicted results do not always match with test results.
In both LCF and HCF, damage phenomena occur in the grains and therefore the use of mesoscopic parameters (stress σ, strain ε,...) seems more relevant than macroscopic parameters (Σ, **E**...) for studying these fatigue phenomena. It is well known that σ and Σ are related by the following relation:

$$\sigma = \mathbf{A}.\Sigma + \rho$$

where ρ is the mesoscopic residual stress field and **A** is the elastic stress localization tensor. The presence of the mesoscopic residual stresses , which depend closely on the characteristics of the loading path, shows that it is in general not correct to use the macroscopic stress Σ to characterize phenomena at the grain scale.
However, the evaluation of the local mesoscopic fields from the macroscopic ones is a difficult task. The material must be considered as locally heterogeneous and has to be considered as a structure when submitted to complex loading histories. Depending from the loading characteristics, one can accept different simplifying assumptions which permit a solution to the problem. We shall suppose that fatigue is related to the possibility of shakedown. Thank to this assumption, which was already proposed in 1963 by D. Drucker, it is possible to propose fatigue criteria which give very good fatigue predictions on real mechanical structures.

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MULTISCALE MODELLING OF LOCALIZATION IN SHEET METALS

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Applications of crystal plasticity theory to the numerical modelling of large strain plasticity phenomena are considered. In particular, instabilities and localized deformation phenomena for FCC polycrystals subjected to various deformation modes are investigated. In-house finite element analyses based on a rate-dependent crystal plasticity model have been developed to simulate the large strain behaviour for sheet specimens subjected to plane strain tension, plane stress tension, simple shear and channel die compression. In the formulation, plastic deformation of an individual crystal is assumed to be due to crystallographic slip. Parallel computing algorithms have been developed for the numerical simulations.

Modelling of the polycrytalline aggregates is carried out at various scales. In some of the simulations, each material point in the finite element analyses is considered to be comprised of a large number of FCC grains, and the Taylor theory of crystal plasticity is adopted to model the behaviour of the polycrystal. In other simulations, one or more elements per grain are modelled. These formulations account for initial textures, as well as texture evolution during large plastic deformations. The results of simulations for the above-mentioned deformation modes are discussed, and in certain cases comparisons are made with experimental results for rolled aluminum sheet alloys. The effects of various parameters such as initial texture and texture gradients on the formation of localized shear band failures are discussed. The importance of modelling at appropriate scales to properly predict localized deformation instabilities is examined.

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Multiaxial plastic fatigue behavior with multiscale Modeling

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A multi-scale model of damaged elasto-inelastic behavior is proposed to predicted the damage evolution during multiaxial plastic fatigue. The fatigue life for FCC metallic polycrystals is evaluated. This model is expressed in the time dependent plasticity for a small strain theory. In this approach, the elastic part, assumed to be uniform, isotropic and compressible, is estimated at the granular scale (meso scale). An intragranular isotropic hardening variable is introduced on each crystallographic slip system (css), while the kinematic hardening effect can naturally be described by a self-consistent interaction law. From physical viewpoint, it is assumed that the damage occurs on the css level, where the slip is highly localized. The model considers that the micro-damage variables initiate and then evolve on the activated crystallographic slip systems. The associated generalized thermodynamic force is determined as an inelastic energy defined only by the intragranular isotropic hardening without the elastic energy contribution. This is different from the macroscopic theory of damaged inelasticity where this associated force includes the elastic energy contribution. The damage variable is coupled with elasto-inelastic constitutive equations at the micro (css) and meso (grain) scales. The quasi unilateral effect is neglected in this approach.
In this work, the model is tested under different multiaxial cyclic loading situations (tension-compression and tension-torsion with 0°, 45°, 60° and 90° out of phase) to show the effect of the loading paths on the fatigue life of polycrystals. The effect of the model parameters on the fatigue life is also studied. Some macroscopic and microscopic numerical responses are recorded and discussed. As a conclusion, the model can appropriately describe the overall and local damaged behavior of polycrystals.

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A model for Damage, Opening and Sliding of Grain Boundaries

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Due to the increasing power of computers and the development of robust integration methods, the polycrystalline behavior can now be investigated by computing realistic aggregates, with a large number of elements to represent the individual behavior of all the grains. This type of calculation has been performed in the last five years at Centre des Matériaux (see for instance [1,2]), with about 200 grains, and 10^6 integration points. This type of study shows that the classical self-consistent approaches are in good agreements with the global mechanical response of the Finite Element model, but, on the other hand, local stress and strain distribution are usually complex: the dispersion is huge, the local distribution does not follow a simple statistical law (Gaussian for instance). The local behavior is affected by the surface, the actual neighbors, and the distance to the grain boundary. The main results of this study, recalled in the introduction, demonstrate also that a good representation of the grain boundary is crucial for the future investigations.

In the past, grain boundaries have been modeled by special elements, or by decohesive zones (Needleman). The present paper proposes a new approach in which the grain boundary itself is a material, with a full set of constitutive equations, allowing elasticity, plasticity and damage. The new development will answer the following questions:
- what are the elastic properties of a grain boundary ?
- what is the proper formalism to introduce damage at the grain boundaries ?
- how can damage affect opening and sliding of the grain boundaries ?

The model is developed in the framework of thermodynamics of irreversible processes. Several propositions are shown, with one or two damage variables, and with several types of coupling between damage and plasticity. The model is implemented in the Finite Element code Zebulon. It is calibrated for representing damage in a zirconium alloy. Several applications are shown, with about 200 grains in generalized plane strains, and also in 3D. The behavior of each grain follows a crystal plasticity model, with several families of slip systems (HCP structure), and the grain boundary is represented by special elements subjected to damage and plasticity. The numerical model is able to correctly represent crack initiation and propagation along the grain boundaries, in a plastically flowing material.

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Gradients of Hardening in Nonlocal Dislocation Based Plasticity

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A thermodynamically consistent framework for the gradient approach in plasticity is proposed. The second order gradient of both the kinematic and the isotropic hardening measures is introduced through the Helmholtz free energy and through the plastic potential function. The macroscale gradients allow one to address the non-local behavior of materials and interpret the collective behavior of defects such as dislocations. The macroscale internal state variable and the corresponding gradient term are assumed to be independent internal state variables with respect to each other with different physical interpretations and initial conditions which allows these two different physical phenomena to be identified separately. The Aifantis-Walgraef dislocation model is used to give micromechanically based definitions for the nonlocal coefficients.

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Global and Local Constraints in the Theory of Compaction of Granular Materials

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In a granular packing subjected to a hydrostatic compressive stress state, consideration of the relation between the overall stress and the intergranular contact forces leads to a global constraint on the selection of the force distribution. If this is the only constraint, then the principle of maximum entropy will dictate the system to behave like a Maxwell-Boltzmann (MB) ideal gas, namely, that the force distribution will follow the simple law $P(\langle f \rangle) = \exp(-\langle f \rangle)$, where P is the probability density, and $\langle f \rangle$ the force magnitude normalized by the mean force value. Many computer simulation and experimental results, however, indicate that P exhibits a maximum at the mean force, and that its exponential decay at large forces is much faster than the MB law. In this paper, it is first argued that forces in a structurally random granular packing in general will not follow the MB distribution, because unlike the molecules in an ideal gas, the forces in a random packing are strongly correlated. Because each grain has to be in equilibrium, the existence of a large force on one grain, for example, will have to be accompanied by the existence of a few other large forces to balance it. There exists, therefore, a "local" constraint, originating from the force correlation on a local scale. The force distribution $P(\langle f \rangle)$ will then have to satisfy both the global and local constraints. In this work, a mean-field approach is applied to investigate the local constraint, and the admissible solutions to both constraints are explored. A common solution is identified, which shows good agreement with computer simulation results.

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Three-Dimensional Structures of the Geometrically Necessary Dislocations Generated from Non-Uniformities in Metal Microstructures

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Development of dislocation structures during deformation has long been studied. On the basis of continuum mechanics analysis, two types of dislocation densities can be evaluated; the statistically stored and the geometrically necessary dislocations. Density increment of the statistically stored dislocations is related to the mean free path of them and the increment of plastic shear strain, while the density of the geometrically necessary (GN) ones is related to the spatial gradient of the plastic shear strain on slip systems.

We use the finite element method to analyze slip deformation in microstructures of f.c.c. type metals and evaluate the edge and screw components of the density of GN dislocations as well as the density norm and the direction vector of the dislocation line segments for all elements in a specimen. After this process, we can reconstruct an image for the three dimensional structure of the GN dislocations in a deformed microstructure.

Some types of microstructures are numerically constructed and the GN dislocations after slip deformation are evaluated. It is well known that loop shaped dislocation structures, called the Orowan loops, are formed after slip deformation in two phase material where inclusions are sparsely distributed in softer matrix. We make some models for such two-phase microstructure where an inclusion of cuboidal, hyper-elliptical, spherical or ellipsoidal shape is embedded in a softer matrix. We apply a uni-axial load to the models and calculate the structure of GN dislocations. The results show that the loop shaped structure is formed around the inclusion and a double-kink-wall type structure develops in the direction perpendicular to the slip plane. In addition to these, small loops are also formed near the hetero interface. GN dislocations in single-phase materials are also studied. In the analysis of tensile deformation of a multi-crystal plate, which includes six crystal grains, primary slip is observed to start in the grain interior and "pile up" of GN dislocations at grain boundaries gradually take place. Slip deformations on secondary systems are also observed, although their activities are confined within a region near grain boundaries. Dislocation structures in single crystal specimen are studied also. The initial flow stresses on slip systems are determined by normally distributed deviates and uni-axial tensile load is applied to the specimen. The results of the analysis show development of wall like structure of dislocations, which extend as wide as the width of the whole specimen.

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Simulation of Texture Evolution in Equal Channel Angular Extrusion of Copper Using a New Flow Field

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Equal Channel Angular Extrusion (ECAE) is a complex deformation path, which is not yet known satisfactorily. Earlier simulations (1,2) used a hypothetical very simplified flow field and were applied to predict the texture evolution in ECAE deformation when the extrusion angle is 90°.

In the present work, a new, more precise flow field is proposed which uses an analytical flow function. The proposed function is inspired from finite element calculations. The velocity gradient that follows from the analysis is incorporated into the Taylor and self consistent viscoplastic polycrystal codes. The evolution of deformation texture is predicted up to 8 passes in the A-route ECAE deformation of copper polycrystal. Self and latent hardening of the slip systems is considered. The predicted textures are in good agreement with experiments.

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Energy Dissipation Mechanisms in Ductile Fracture

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The objective is to investigate energy dissipation mechanisms that operate at different length scales during fracture in ductile materials. A dimensional analysis is performed to identify the sets of dimensionless parameters which contribute to energy dissipation via dislocation-mediated plastic deformation at a crack tip. However rather than use phenomenological variables such as yield stress and hardening modulus in the analysis, physical variables such as dislocation density, Burgers vector and Peierls stress are used. It is then shown via elementary arguments that the resulting dimensionless parameters can be interpreted in terms of competitions between various energy dissipation mechanisms at different length scales, for example between dislocation nucleation from a crack tip and dislocation nucleation from a Frank-Read dislocation source in the material close to the crack tip. Criteria are established which are used to determine the initial, and perhaps dominant, energy dissipation mechanism at a crack tip. The predictions compare favorably with known fracture behavior of a large class of materials.

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CONSTITUTIVE MODELING OF VISCOELASTIC UNLOADING OF GLASSY POLYMERS

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A great number of studies dealing with constitutive viscoelastic modelling of glassy polymers has been published. A large part of them present good results for simulation of polymer structures under various loadings as tension and compression tests, creep and relaxation tests, and take into account the microstructures properties [1], [2], [6, 7, 8], [10]. However, the simulation of unloadings to free stress after tensile loading cannot be obtained by classical rheological models. In particular, constitutive modelings based on Maxwell viscoelastic equations underestimate largely the velocity of the strain recovery, even in case of small deformation. This phenomenon is quite similar in case of using Zener constitutive law, or generalized Maxwell or Zener modelings and all combinations of these approaches. Using a finite number of relaxation times in that case does not be sufficient to increase the recovery strain velocity as necessary, when the viscoelastic parameters are identified on the positive strain rate part of the behavior. Similar results and observations can be obtained with loadings and unloadings displaying strain rate jumps ; in that case, the defaults of the classical modelings are particularly increased.

In the framework of local state method [3], [4], we study the possibility to modelize strain rate jumps and unloadings to free stress for glassy polymers. An extension of the Sokolovski-Malvern equation can be built up [5], [9]. This approach permits to define a function of strain, characteristic of the material, and non dependent of the strain rate. With this function, approximated by a polynomial function of strain, the single internal variable is implicit and can be eliminate writing the constitutive law, and deriving the potential. For classical polyolefins as polyethylene or polypropylene, the evolution of the strain rate jumps can be modelized with a good accuracy under positive or negative strain rates. In that case, the constitutive equations built up can be interpretate as a generalization of the Zener approach in terms of thermodynamically considerations and can be used for different kind of materials.

Unfortunately, the unloading behaviors depend also on the identification of the viscosity obtained with positive strain rate. The generalization of the Zener modeling taken into account above, permits to separate the signus of the strain rate, but only with artificial considerations unbased on physical properties of materials. With a range of different experimentations, we show that the viscoelastic constants of the glassy polymers tested are necessary different in case of positive strain rate or negative strain rate. Then, different possibilities of physical approches are studied and permit to complete the constitutive laws of glassy polymers.

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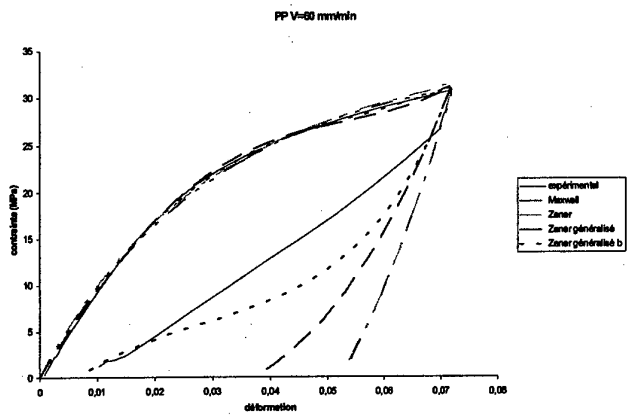

Figure 1 : Polypropylene unloading modelings in comparison with experimental result

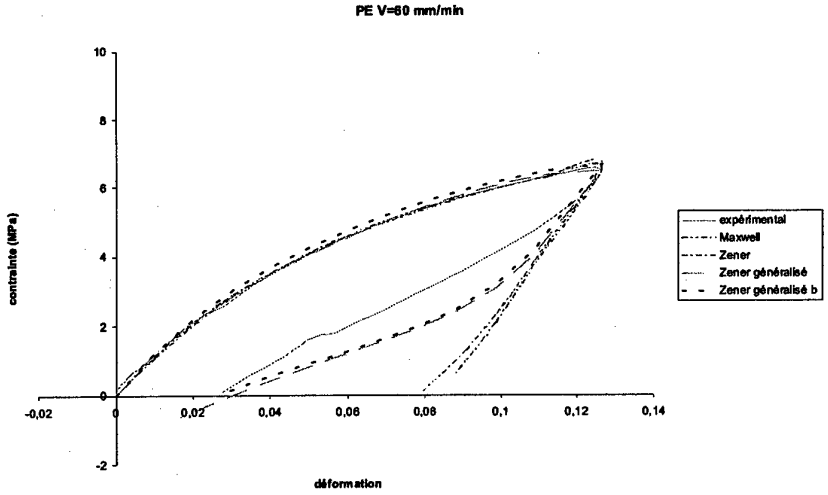

Figure 2 : Polyethylene unloading modelings in comparison with experimental results

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A Microcracking and Spall Based Model to Describe the Dynamic Response of for Brittle Materials under Shock and Penetration Loading

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Ceramic materials exhibit inelastic behaviors due to microscopic deformation and fracture processes under impact loading conditions. Ceramic damage is often due to microcrack nucleation, growth, and coalescence. A microcracking model based on both spall and Griffith criteria was used to describe crack damage evolution in the ceramic. The spall criterion assumes that rapid microcrack growth occurs (at a rate equal to the Rayleigh wave speed) when all three principal stresses are positive (tension) and the largest principal stress exceeds a critical value (spall strength). When damage accumulation due to spall was added to the microcracking based model, realistic predictions of measured velocity and stress histories were achieved for a wide range of stress/strain states. This paper presents results from numerical simulations of shock wave and projectile penetration experiments on a brittle ceramic material.

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On the constitutive theories of power-law materials containing voids

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The constitutive theory of incompressible power-law creeping (or time independent plastic) solids containing distributed porosity is investigated. The voids are assumed to be spherical and arranged in a space filling cubic array. A thick-walled spherical shell in which the void is traction free is taken as a representative volume element (RVE). Both uniform traction and linear velocity boundary conditions are prescribed on the outer surface of the RVE in modeling the remote fields. The numerical solutions are obtained accurately and effectively using a Ritz procedure based on Hill's minimum principle of the velocity. Two constitutive laws based on uniform traction and linear velocity boundary conditions are proposed. The proposed constitutive laws are also used to evaluate several existing constitutive laws of power-law creeping solids containing voids.

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objective quatification of the ductility within the coupling elasticity-damage behavior : FORMULATION

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The mechanical behavior of a material is never purely elastic and linear. In fact, many intrinsic phenomena occur and render it to a macroscopic scale non linear. The amplitude of this non linearity informs whether the material is fragile or ductile.
In fact, the ductility of a material represents its aptitude to bear deformation under external loads without breaking. In fact, it determines the level of cohesion between the particles of the material to be enough linked one to another. But, its quantification is quite difficult particularly for the heterogeneous materials presenting non linear behavior.
The importance of determining the ductility is also due to the fact that it is directly related to the deformation of the material which is admitted to be a source of the crack. Indeed, the crack is consecutive to an overflow of the strain or to a limitation of the strain which then induces stresses that cause fissures.
Another phenomenon of great importance, that is related to strain, is the interface block-mortar which is known to be the weakest element of the masonry. A better understanding of the deformation and consequently the ductility of each of the block and mortar is fundamental to know more about the interface and then to optimise its strength.

This work deals with a mechanical behavior based on coupled elasticity-damage where a corrective term is added to linear elasticity to take into account the state of deterioration occurring in the material. This deterioration goes along with the deformation process and happen apparently in decreasing the strength.

Herein, the ductility is quantified by the ductility factor expressed as the ratio of the limit constraint to the elastic constraint. This ratio is then explicitly developed to be found written only by the damage coefficient as a correcting term.

With this formulation we are able to quantify objectively the ductility of a material with an elastic-damage coupling behavior. Representing a ratio of strains, the factor of ductility is found simply depending of the coefficient of damage. The latter was introduced to correct the elastic behavior of the material. This ratio will be of a simple and a standard use in engineering.

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A New Model for Dilational Plasticity and Applications to Ductile Solids

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A micromechanical framework is developed that accounts for various modes of dilational plastic flow in rate independent solids assuming normality in all. The model is defined by a set of constitutive equations including a closed form of the yield surface along with appropriate evolution laws for microstructure-based internal variables. The framework is applied to model coalescence of voids in ductile solids on micromechanical grounds [1].The derivation of the evolution laws is carefully guided by coalescence phenomenology inferreed from unit-cell calculation and detailed experimental investigations. The relevant internal variables are the void shape and aspect ratio, ligament size and void orientation. The major implication of the model is that the stress carrying capacity of the elementary volume vanishes as a natural outcome of ligament size reduction. Moreover, the drop in the macroscopic stress accompanying coalescence can be quantified for many initial microstructures provided that the microstructure state is known at incipient coalescence. The model is suitable for finite-element implementation and indications are given as to how to effectively use the model in a predictive approach.

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Influence of temperature and loading rate on the characteristics of PLC bands in an Al-Mg alloy

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Within a certain regime of temperature and loading rate, serrations or stairs in the flow stress occur during deformation of alloys containing interstitial or substitutional solutes. The occurrence of these serrations (stairs) is generally known as the Portevin- Le Chatelier effect. Each stair or serration corresponds to the nucleation and/or propagation of a deformation band along the tensile specimen. Microscopically, the PLC effect is associated with dynamic strain ageing due to transient interactions between mobile clouds of impurities (diffusing solute atoms) and glide dislocations.
Tensile tests of aluminium-magnesium alloy (5182 O) were performed in a wide temperature range under various constant loading rates to investigate the effect of testing temperature and loading rate on PLC plastic instabilities.
Experimental results show a closing of the domain where PLC effect occurs, in $\log\dot{\varepsilon}$ (or $\dot{\sigma}$) versus $1/T$ diagram, towards high temperatures and loading rates. This result is in qualitative agreement with recent theoretical results by Hähner based on a physical model of dynamic strain ageing.
The conditions for the occurrence of normal and inverse behaviours of the critical strain, ε_c, for the onset of repeated yielding, are derived. Indeed, ε_c increases with increasing loading rate and/or decreasing temperature in the normal behaviour domain, while the inverse effect, which is characterized by a decreasing critical strain with increasing loading rate and/or decreasing temperature, has been observed at low loading rates. Moreover, the stress drop evolution shows a negative strain rate dependence with two slopes close to (-0.2) at low strain rates and (-0.75) at high strain rates.
The effect of specimen surface finish on the band propagation velocity V_b under stress control was investigated. The tests results show that bands may propagate about twice as fast in the polished specimen as compared with the unpolished sample. It is important to note that he variations of V_b as function of $\dot{\sigma}$ for different temperatures show a decrease when $\dot{\sigma}$ increases. This result is in quantitative agreement with the results obtained by Hähner that are based on a gradient-dependent generalization of the dynamic strain ageing kinetics.

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Planar impact simulation for ductile metals

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It is well established that high rate failure of structural materials takes place by rate processes occurring at the micro level and involving nucleation, growth, and coalescence of voids or cracks. At submicroscopic level, the mechanism of failure in polycrystalline materials is often dislocation controlled. The process of deformation and failure can be therefore described by plastic glide, which involves the mechanism of dislocation pile-ups. To describe these processes in planar impact (cylindrical and conical target) of ductile metals, the dislocation based constitutive plasticity model, the Mechanical Threshold Stress (MTS) model, along with the void nucleation and growth (NAG) model are implemented in the finite element code ABAQUS/Explicit. The porosity of the material is noted by:

$$f_v = \frac{V_T}{1+V_T}$$

with

$$V_T = V_0 + \sum_t \Delta V_N^{new} + V_{CG}$$

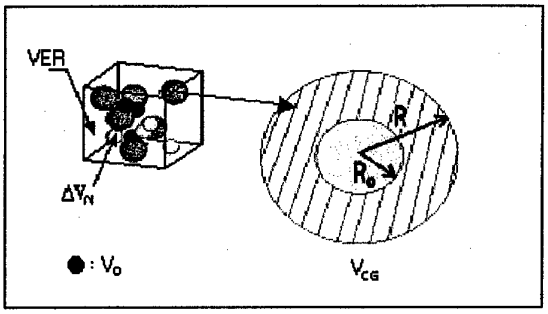

Fig. 1. Nucleation and growth of voids

where, f_v is the porosity in the material, V_T is the total relative void volume, V_0 the pre-existing relative void volume, ΔV_N^{new} corresponds to the relative void increment by nucleation during the time increment Δt and V_{CG} is the relative void volume of the crown obtained by growth (see Fig. 1.).
We perform numerical simulations of planar impact test with various target geometries. We studied the influence of the boundary conditions on the damage map in the target. The material used for these simulations is OFHC copper. Our predicted results are compared with experimental ones.

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Validation of the tangent approach for the solution of the non-linear Eshelby inclusion problem

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A fundamental problem in micromechanics is to calculate the local strain or strain rate in a heterogeneous material in terms of the overall applied strain or strain rate. For that purpose, the solution of the Eshelby problem appears as a crucial step. Eshelby (1957) has considered an ellipsoidal heterogeneity embedded in an infinite matrix. The material is linear elastic. The tensor of elastic moduli is uniform within the ellipsoid and uniform within the matrix. A closed form solution was proposed in which the strain within the ellipsoid was calculated in terms of the applied macroscopic strain. A remarkable outcome of this solution was the demonstration of strain uniformity in the ellipsoid.

An extension of the Eshelby problem for non-linear viscous materials is considered. An ellipsoidal heterogeneity is embedded in an infinite matrix. The material properties are assumed to be uniform within the ellipsoid and in the matrix. The problem of determining the average strain rate in the ellipsoid in terms of the overall applied strain rate is solved in an approximate way. The method is based on the non-incremental tangent formulation of the non-linear matrix behavior (Molinari, A., Canova, G. R., Ahzi, S.). Note that the strain rate in the inclusion I obtained with this linearization procedure, is uniform within I. However, when non linear material responses are considered, the real strain rate distribution is non uniform in I. The comparison made with finite element calculations will indicate to what extent the hypothesis of strain uniformity within I is violated.

In the present work this approximate analytical solution is compared to finite element calculations for various inclusion shapes and loading conditions. Non-linear viscous responses are considered. A localization law is obtained by approximating the non-linear response of the matrix with the tangent response in the vicinity of the macroscopic applied strain rate.

The scope of this paper is to validate the approximate analytical solution by comparison with the results of finite element calculations (Gilormini and Germain (1987); Gilormini and Michel (1999) and Molinari; El-Houdaigui and Toth (1999)). Various aspect ratios of the ellipsoidal inclusion, different hardness ratios for the material in the ellipsoid and in the matrix, several loading paths and different strain rate sensitivities are considered.

The tangent approach appears to give a good approximation of the solution, as long as the comparison is made with the averaged value of the strain rate within the inclusion. It can be seen that the flow heterogeneity within the inclusion tends to increase when the strain rate sensitivity is small.

The advantage of the present non-incremental tangent treatment of the non-linear inclusion problem is that all mathematical conveniences of the linear Eshelby solution are retained.

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On plasticity and Damage Evolution During Sheet Metal Blanking

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To correctly simulate the blanking process of thin metallic sheets at different stroke rates, it is necessary to use material models which account for microstructural effects as well as the effects of loading conditions. These models should couple plasticity and damage evolution up to failure. In this work, we investigate the blanking process using models accounting for high stroke rate (leading to high strain rate) such as the Johnson-Cook model for plastic flow and failure. We also propose a new damage model for ductile failure based on the continuum damage mechanics (CDM) formulation. This model is based on the hypothesis that a damage dissipation potential exists and is a non linear function of the effective cumulated plastic strain.

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Thermo-electro-elastic effective properties of piezoelectric composite materials

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Presented here is a thermo-electro-elastic modeling of effective properties of piezoelectric composites containing spatially oriented inclusions. Extension of the heterogeneous inclusion problem of Eshelby for elastic to electro-elastic behavior is formulated in terms of four interaction tensors. These tensors are basically used to derive the self-consistent model, Mori-Tanaka and dilute approaches for ellipsoidal piezoelectric inclusions. Solutions are based on numerical computations of these tensors for various types of inclusions [1]. Using the obtained results, effective thermo-electro-elastic moduli of piezoelectric multiphase composites are investigated by an iterative procedure in the context of self-consistent scheme. Generalized Mori-Tanaka's model and dilute approach are re-formulated and used in the analysis. Multiphase composites with reinforcement ranging from spherical particles to continuous long fibers randomly distributed at fixed spatial orientations are analyzed. Influences of the pooling direction, volume fraction, shape of the inhomogeneities on the elastic moduli, piezoelectric, dielectric and pyroelectric coefficients are investigated for various types of piezoelectric composite materials.

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Size Effect of Fine Structures - Experiments and Theory

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The mechanical elastic properties of fine structures in micron and nanometer scales are size dependent. Experiments in bending of walled nanocarbon tubes have shown that the tube stiffness can increase by nearly ten times of conventional expectation
when the size of the tube is decreased from 40 nanometers to 8 nanometers. The stiffness of micron-scaled epoxy beams has been shown to increase by three times when the beam thickness is reduced from 115 microns to below 20 microns. The stiffening has been attributed to the stiffening effects of strain gradients based on higher order elasticity theory. The higher order theory involves elastic material parameters in addition to the two in the classical theory for isotropic materials. Such mechanical behavior is important in micro- and nano-electromechanical systems and in optoelectronic applications.

Elasticity theories including the rotational gradients in the constitutive equations were developed in 1960s. Mindlin (1965) developed a general higher order stress theory to explain the size effect. Fleck and Hutchinson (1997) reformulated the theory and renamed it the strain gradient theory. We derived a modified strain gradient theory of elasticity with an alternate decomposition of the second order deformation gradient tensors. The additional material parameters of the higher order deformation theories manifest as the size effect.

We have established the beam bending and torsion solutions to identify the strain gradient contributions to the bending and torsion rigidities as a function of structural size. The size effect has been confirmed by experiments using epoxy. The confirmation of the significant elastic strain gradient effect by theory and experiments opens up a new frontier in the study of elasticity in micron- and nanometer-scaled structures.

In this report, we shall also investigate the physical basis of the strain gradient stiffening in fine structures using molecular deformation model. We shall examine the effects of three bodies and higher molecular interactions on the size dependence in bending. The relation between molecular origin of stiffening and strain gradients in continuum mechanics will then be discussed.

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Influence of microstructural parameters on shape memory alloys behavior

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Modeling the functional behavior of material undergoing a martensitic phase transformation like in shape memory alloys (SMA) is a challenge for the development of industrial applications using these materials. Multiscale modeling concepts developed in mechanics of materials are very well adapted to solve this problem.
The formation and growth of the different variants of martensite at the crystal level are derived using thermomechanical approach. . At this point the more difficult aspect is the description of the different classes of interaction, which are observed between martensite variants. The use of interfacial operators allows solving this problem and lead to the definition of an interaction matrix.
Two examples of how the intergranular interactions build during the transformation in polycrystalline materials are described for bulk material and thin film.
Evolution of different microstructural parameters are presented and discussed.

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Analysis of Ridging in Ferritic Stainless Steels Using Crystal Plasticity Finite Element Method

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The crystal plasticity finite element method (CPFEM) is one of the most powerful simulation tools, which can take the orientation and microstructure of material into account. The purpose of this study is to investigate the effects of texture and microstructure on the macroscopic anisotropy from micromechanical point of view using CPFEM. The ridging problem in ferritic stainless steel (FSS) has been well known and unsolved for more than three decades. FSS sheets exhibit ridging parallel to the rolling direction when subjected to tension or deep drawing. The origin of ridging behavior has not been clearly explained yet. Many people agree that ridging originate from different plastic anisotropies of grains. In this study, STS430 and STS409L stainless steels having columnar and equiaxed structures were chosen as initial specimens to elucidate the role of microstructure and composition on ridging. The specimens having initially the columnar structure show severe ridging and STS409L stainless steels show a worse surface quality. The existence of band-like colonies of similar orientations was found in the center of the sheets by EBSD measurement. In addition, the previous models suggested by other researchers were examined quantitatively by CPFEM. The results simulated based on the model suggested by Chao and Wright were different from their predictions. In order to obtain a more realistic ridging simulation, the specimens containing variously oriented colonies in a γ-fiber textured matrix were also considered. The simulated results showed that the lower plastic strain ratio of {001}<110> colonies and different shear deformations of {111}<110> or {112}<110> colonies resulted in ridging.

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Grain-Boundary Effects and Ductile Failure Evolution in Crystalline Aggregates

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Dislocation-density based inelastic crystalline formulations and specialized computational schemes have been developed to characterize material failure on the relevant physical scales needed for the accurate prediction of physical mechanisms that control failure initiation, growth, and coalescence. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and tilt orientations. These evolving local stress fields are used as failure criteria to track the initiation and evolution of intergranular and transgranular fracture. The interrelated effects of grain boundary orientation, dislocation density pile-ups and evolution, geometrical and thermal softening, void distribution and geometry, and hydrostatic stresses on failure paths in cubic crystalline materials have been studied. Based on the present analysis and on comparison with experimental observations, it is shown transgranular and intergranular failure can be characterized in terms of the competition between the strengthening and the softening mechanisms of the crystalline structure.

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Particles cluster effect on the damage and failure of metal-matrix composites : micromechanical approach

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Metal-matrix Composites (MMCs) have been developed in order to combine the following properties : stiffness of the reinforcement, with the high ductility and fracture toughness of the matrix. They constitute a very attractive range of materials particularly for aeronautical structures looking for performance improvement as well as structure integrity. Our objective is to predict the anisotropic tensile behavior, the damage evolution up to failure of these composites as a function of their microstructure. We are interested in aluminum alloys reinforced by different volume fraction of silicon carbide particles. The materials were made by a powder metallurgy extrusion. Some of them have been deliberately manufactured with clusters of particles by mixing an aluminium's powder with a composite's powder.

We present multi-scale modeling of the damaged plastic behavior and failure of Al/SiCp composites. We study the influence of an heterogeneous dispersion of the reinforcement (volume fraction, aspect ratio, orientation) on the damage development and the failure strain of composites. We consider that a composite which contains a cluster with a higher volume fraction of reinforcement, results on the association of two homogeneous micro-composites. Each one is modeled by Mori-Tanaka's approach; we choose the homogenization by the self consistent model for the blend of these micro-composites.

Particle cracking is the principal source of damage and we use a Weibull law in order to define the evolution of the volume fraction of broken particles. The statistical development of damage is introduced in the elastoplastic behavior law. The first stage of a failure criteria definition is to determine the range of stress and strain fields in the matrix close to the SiC broken particles, in accordance with the composition of the elementary volume and the macroscopic plastic strain. At the second stage we determine the growth rate of cavities initiated on the precipitates in the matrix. The linking of the micro-cracks depends on the value of the growth rate and on the distance from the crack where this critical growth rate is obtained. The strain distribution near the crack is determined from the Hutchinson, Rice and Rosengren solution. Ligament failure arises when the growth rate becomes critical on a distance equal to half of the distance between two broken particles (C-C arrangement). The failure strength of a composite material is related to the defects present in the material and the heterogeneous distribution of the reinforcement.

We have demonstrated that the particle clusters in a material could control the failure strain.

Particles cracking is less important in the clusters, however distance between cracked particles increased the localisation failure in the matrix. These results are in accordance with previous experimental observations.

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A COHESIVE SEGMENTS APPROACH FOR CRACK GROWTH

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In conventional engineering fracture mechanics, crack growth is assumed to occur by the extension of a single dominant crack. However, there are a wide variety of circumstances where the fracture process involves the nucleation and growth of multiple crack-like flaws. For example, in heterogeneous materials, multiple cracks may initiate and grow in one phase which then link up by nucleating cracks in another phase or by propagating across phase boundaries. Another example is the transition from subsonic to intersonic crack speeds via the nucleation of a micro-crack ahead of the main crack. Also, in quasi-brittle materials micro-cracking in front of the main crack tip plays a key role in setting the fracture toughness. Hence, a need for analysing discontinuous crack growth arises in a wide variety of contexts.

Discontinuous crack growth can be modelled within a cohesive surface framework. Within such a framework, constitutive relations are specified independently for the bulk material and for one or more cohesive surfaces. The cohesive constitutive relation embodies the failure characteristics of the material and characterises the separation process. Fracture, if it takes place, emerges as a natural outcome of the deformation process without introducing any additional failure criterion. Furthermore, from dimensional considerations, a characteristic length is introduced.

Methods where cohesive surfaces (or zones) are incorporated into continuum finite elements using the partition-of-unity property of finite element shape functions are available. In these approaches a crack is regarded as a single entity. Here, we describe a cohesive finite element method based on the partition-of-unity property that is applicable when crack growth is discontinuous. The crack is not regarded as a single entity. Instead, it is modelled as a collection of overlapping cohesive segments. The combination of overlapping cohesive segments can behave as a continuous crack. In addition, since cohesive segments can occur at arbitrary positions and at arbitrary orientations, the method allows for complex crack patterns to emerge. Numerical examples illustrating characteristic features of the methodology are presented.

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Atomistic simulations of materials deformation at high-strain rate

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We report the results of atomistic simulations to provide mechanistic insight into the dynamic response of materials to shock loading. In particular, we address outstanding questions regarding the terminal dislocation velocity at high strain-rate, the detailed atomistic mechanisms of twinning deformation modes and the activation of dislocation sources in Al and Cu at high-strain rate. Molecular dynamics (MD) simulations directly account for core interactions through semi-empirical interatomic potentials and provide fundamental insight into dislocation migration and material deformation mechanisms. Furthermore, the length, timescales and strain rates accessible in atomistic modeling by MD are directly comparable to those probed in experiments. This presentation will focus on recent MD simulations of the mobility of edge dislocations at Al and Cu at high-strain rates, the atomistic mechanism of twin deformation and the operation of dislocation sources.

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HOMOGENIZATION TECHNIQUES BASED ON STATISTICAL CONTINUUM APPROACHES

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This paper focuses on the application of statistical continuum mechanics for the prediction of effective properties and their evolution in a heterogeneous media. An analytic form of two-point probability distribution function suitable for general case of two-phase composite medium is introduced and compared to the distribution of phases in a computer generated microstructure. A computer image processing analysis is used to capture the nature of the distribution function. Conditions for the degree of randomness and periodicity are discussed with respect to the new parameters in the distribution function. Mechanical properties of heterogeneous materials are highly dependent on the constituents' configuration and their distribution. The distribution and morphology of the microstructure is represented by two and three point probability functions. The strain rate is taken to be proportional to the resolved local shear stress raised to a power. In the case of elasticity, contributions to the strain rate due to elasticity are neglected and a Green's function solution is derived for the two isotropic media. A two-Green's function solution to the equations of stress equilibrium, originally proposed by Molinari, et al., is utilized to obtain the constitutive law for the heterogeneous medium. This relation links the local velocity gradient to the fields of the local viscoplastic modulus and the imposed strain rate. The concepts of statistical continuum theory are introduced into the localization relation to obtain a closed form solution. The resulting model calculates an effective modulus for the two-phase composite medium (elastic or plastic). Numerical results are presented which describe the evolution of certain morphological features of the microstructure.

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MICROSTRUCTURE DESIGN FOR POLYCRYSTALLINE MATERIALS

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Advances in the spectral methodology for microstructure design of polycrystalline materials are described. The microstructure hull, consisting of all possible microstructures within a specified mechanical/physical framework, is described in Fourier space. It is shown that first-order bounding relationships and estimates for elastic and plastic properties are represented in this space by hyper-surfaces that intersect the microstructure hull. Thus, the objectives and constraints of the design engineer can be represented by a set of surfaces that define a subregion of the microstructure hull. Appending local state variables other than crystallite orientation (e.g., composition, reference shear stress, etc.) is permitted. Application of the methodology to the design of microstructures that decrease notch sensitivity is described. Extensions of the methodology to higher-order descriptions of microstructure is illustrated in the case of the 2-point correlations of local state.

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Reaction-Diffusion Approach to Self-Assembled Nanostructure Formation in Thin Films.

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Thin films play an important role in a wide number of industrial applications, and, in particular, in electronic manufacturing of integrated circuits. It is then of capital economic and scientific interest to understand and master thin film growth, since growth mechanisms usually determine film properties and textures. As a result the modeling of thin film growth has been one of the most active research areas, since the 1950's. With the dramatic increase of computer capabilities, numerical simulations were carried out some twenty years later. Numerous computer simulation methods have been developed to study growth of thin films since the 1970's. These investigations not only improved existing theories, but also revealed detailed information, such as island shapes, step formation and surface roughening of a growing thin film. However, due to their atomistic nature, they can deal only with small systems, with linear dimension under the micron. It is why continuum approaches are of great interest, since they are capable of simulating growth of thin films of larger dimensions. Such models have been proposed to describe mesoscopic scales, in order to improve the understanding of deposition processes and film surface evolution at a scale inaccessible by both traditional equipment (macroscopic) and feature scale (microscopic) models.

Continuous models have also been proposed to describe the spontaneous ordering of nanostructures or self-assembled quantum dots in multicomponents epilayers on a substrate. They are based on an underlying instability of the alloy or solid solution which form the film. In this case, when the solid solution is unstable, below a critical temperature, it undergoes spinodal decomposition, which leads to phase coarsening. On the other hand, concentration-dependent surface stress or atomic deposition on the surface drive phase refining. As a result of the competition between these two effects, the phases sometimes select stable, nanometric, sizes. Furthermore, they may order into periodic patterns, such as alternating stripes or disks lattices. However, in these models, the films are already well developed, and growth or kinetic processes, such as atomic deposition and reaction are not considered.

Here, a reaction-diffusion scheme, which takes into account adsorption, desorption and nonlinear diffusion, is proposed, to describe the evolution of a deposited atomic layer on a substrate. It is shown that, either in monocomponent films and solid solutions, the competition between atomic deposition and the underlying instability of the adsorbed atomic layer may stabilize nanoscale spatial patterns, already in the first deposited layers. These patterns may serve as templates for the late stages evolution of film textures. Patterns with different symmetries may be selected, according to the relative values of experimental parameters such as deposition rate, substrate temperature and atomic mobility. Furthermore, for low deposition rates, patterns may change with time, according to the evolution of the mean surface coverage. In this approach, self-assembled nanostructures appear as dissipative structures, and their selection and stability mechanisms are of dynamic nature, in agreement with the experimental situation, and in contrast with other approaches, where selection results from the minimization of a free energy. It is also shown that the effect of texture evolution, grain orientation and internal stresses may easily be incorporated in this description.

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Multi-axial Behavior of Polycrystalline Shape Memory Alloy and Its Constitutive Equations

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The main mechanism of shape memory alloy is the martensite phase transformation and its reverse transformation (the austenite phase transformation). These two phase-transformations are controlled by the applied stress and temperature. Till now, almost all research works on the mechanical behavior of shape memory alloy were conducted under the simple thermo-mechanical loading condition, for example, the uni-axial tension test at the constant temperature, and thus the mechanical behavior of shape memory alloy under the complex thermo-mechanical loading conditions (that is, the multi-axial complex loading and the change of temperature) are still quite unknown. From this point of view, the authors have investigated the mechanical behavior of shape memory alloy under the thermo-mechanical complex loading conditions by applying the combined loads of axial force and torque to the thin-walled tube specimen, and several interesting and unique phenomena were observed. Also, these phenomena were discussed from the micro-mechanical point of view. In this paper, the formulation procedure of general constitutive equations which can predict these unique behaviors is described briefly, and the predicted results are compared with the experimental results. The formulation procedure of the constitutive equations is based on the following ideas related with the multi-scale (from micro to macro) structure of material.

(1) the formulation of relation between the shear stress-strain of phase transformation variant in the crystal grain component,
the formulation of stress-strain relation of the crystal grain component having several numbers of variants (here, some interactions among the variants are considered), and
the formulation of stress-strain relation of the polycrystalline metallic materials composed of numerous crystal components (here, some interactions among the crystal grains are incorporated).

Keywords: shape memory alloy, constitutive equations, multi-axial loading condition, crystal plasticity, intelligent materials systems

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Mesoscopic Simulations of Easy-Glide and Stage II Hardening of Single Crystals

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Computational studies of plastic flow phenomena arising from the collective motion of a large number of dislocations are carried out by combining dislocation dynamics with a finite element procedure to solve boundary value problems. The current formulation is two-dimensional for computational reasons. However, the physics of three-dimensional dislocation interactions is key to understanding the hardening of single crystals and plasticity at the micron scale. A framework has been developed to account for 3D physics, such as line tension and junction formation, within the 2D computational formulation. This framework is used to simulate forest interactions and strain hardening in single crystals subject to plane strain tension. The basic properties discussed are the conditions under which sessile junctions form, the strength and stability of these locks, and the circumstances under which dislocation intersections result in the operation of new Frank-Read sources. At the relatively large strains reached in the simulations, dislocation storage is stabilized, giving rise to linear second stage hardening and to the formation of rough dislocation cells. A variety of crystal stress-strain responses are obtained and compared with available experimental results.

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Prediction of Damage in Randomly Oriented Short Fiber Composites by Means of A Continuum Damage Mechanics Approach[1]

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When a short-fiber composite structure is submitted to increasing loading, two main damage mechanisms have been observed: *matrix cracking and fiber matrix debonding leading fiber pull out.* These damage mechanisms and their chronology during material deformation have been identified by Meraghni et al. [1-2].

In this paper, a micro-macro approach using continuum damage mechanics is adopted to determine the macroscopic response of a randomly oriented short-fiber composite suffering from matrix cracking. First, the homogenized elastic properties of the virgin composite are computed using *micromechanical models*. Then, the *self-consistent model* by Laws et al. [3] is used to determine the stiffness reduction of an aligned short-fiber composite subject to matrix cracking. The *associated damage variable* is defined as a measure of the crack density. Considering moderate crack densities and assuming completely random and planar orientations of microcracks and fibers, the stiffness of a cracked randomly oriented fiber layer is obtained by averaging the stiffness of a cracked aligned fiber composite over all possible orientations and weighted by an orientation distribution function. Next, to determine the macroscopic response, we extend the *continuum damage mechanics approach* proposed by Renard et al. [4] for unidirectional continuous fiber composites to randomly oriented short-fiber composites. This approach relies on the construction of a thermodynamic potential and a damage threshold function. Furthermore, it is shown that the stiffness reduction law can be fitted by the functions of a form exponentially decreasing with the damage variable. This form was proposed by Renard et al. [4] for continuous fiber composites subject to matrix cracking and can be used here for short-fiber composites [5]. The constitutive equations and thermodynamic force associated with the damage variable are derived from the thermodynamic potential. Finally, using a damage criterion dependent on the damage threshold function, the damage evolution law is obtained by means of the consistency condition.

This damage model has been implemented in the Marc finite element code by means of user subroutines of Marc. The model validation is conducted through the simulation of the uniaxial stress-strain responses of some randomly oriented glass/epoxy composite systems. The numerical predictions will be compared with the experimental results from Meraghni et al. [1].

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NONSTEADY PLANE-STRAIN IDEAL PLASTIC FLOW CONSIDERING ELASTIC DEAD ZONE

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Ever since the ideal forming theory has been developed for process design purposes, application has been limited to sheet forming and, for bulk forming, to two-dimensional steady flow. Here, application for a non-steady case was made under the plane-strain condition. In the ideal flow, material elements deform following the minimum plastic work path (or mostly proportional true strain path) so that the ideal plane-strain flow can be effectively described using the two-dimensional orthogonal convective coordinate system. Besides kinematics, schemes to optimize preform shapes for a prescribed final part shape and also to define the evolution of shapes and frictionless boundary tractions were developed. Discussions include the issues on the elastic dead zone and numerical calculations made for an automotive part under forging.

Key words: ideal forming, plane-strain, characteristic method, rigid-perfect plasticity

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ROLE OF DEFORMATION TWINNING IN MECHANICAL RESPONSE OF FCC AND HCP METALS

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Deformation twinning has been known to play a significant role in the mechanical response of hcp metals (e.g. Ti alloys) and low stacking fault energy fcc metals (e.g. Brass). Our recent experimental investigations have provided tremendous insight into the physics of how deformation twins influence the mechanical behavior of these metals. Although there are major differences in the driving factors for the formation of deformation twins in these two distinctly different classes of materials, the consequence on the mechanical behavior shows remarkable similarity in several aspects. These results will be interpreted in this lecture, and the implications of these results on the modeling efforts will be discussed.

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Multiscale Modelling of Non-linear Behaviour of Heterogeneous Materials: Comparison of recent homogenisation methods

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In various application domains the last decade has shown an increasing need for improved inelastic modelling and lifetime predictions in critical structural components, more and more made of composite materials. Phenomenological methods, which consist of a macroscopic description of experimental observations, using the thermodynamic framework, have been mainly used until the eighties to describe the constitutive behaviour of such heterogeneous materials. Over the past few years, progress in experimental micro-analysis have led to an increasing amount of research works on multi-scale modelling. This particular has the advantage to provide both the local and the overall mechanical behaviour of heterogeneous structures. This article lies within this context by presenting the application of several micro-macro procedures commonly used or recently developed to predict the overall behaviour of non linear composites and polycrystals.

The first approach presented here is based on the idea of a purely elastic redistribution of the macroscopic stress and strain, and of the local eigenstresses or eigenstrains. In this method, initially proposed by Dvorak, the plastic strain is considered as a given eigenstrain. The local stress field is then determined from the fields of eigenstrain

by solving linear problems with eigenstrains and the plastic strain field is updated by the flow rule. First are presented the main lines of the transformation field analysis namely some of its properties for two-phase and

multiphase exploitations. It has long been recognised that the application of the method for a two-phase material deliver very stiff responses. The model can be accurate provided each phase is subdivided into subdomains where the plastic strain is assumed to be uniform. In this case, the method gives accurate results together with a long computing time. In order to avoid this, we propose to use a methodology of "reduction of sub-volumes" in the TFA method. It consists in determining the strain concentration factors and the transformation influence functions introduced in the TFA model and derived by solving a set of linear elastic problems, for an important number of sub-volumes. A transition from a high to a lower number of sub-volumes is then done by using an analytical averaging procedure. Its validity together with its application on various cases are reviewed and discussed in the paper. A particular accent has been put on the definition of the sufficient number of sub-volumes that have to be considered for a correct approximation of the local fields and a correct description of the overall behaviour.

The second class of approaches presented here are based on a linearization of the local constitutive laws. This linearization allows to build a "linear comparison medium" capable of describing the effects of the non-uniformity of the local fields. We first recall the Hill's incremental formulation based on the use of instantaneous or "tangent" moduli or compliances relating the stress rate and strain rate tensors at both the local and the global scales within a step by step homogenisation procedure. Then, the

alternative "affine" formulation, developed by Zaoui and co-workers, is presented. This method based on a linear thermoelastic comparison medium uses the same elasto-plastic tangent operator than the Hill's approach but associated with a non incremental definition of the local non-linear behaviour.
Finally, all these different schemes are applied to predict the overall behaviour of metal-matrix composites. We will discuss the limitations and the advantages of these procedures together with comparisons to simulations performed by the Finite Element Method. A particular accent is put on the choice of using the correct anisotropic formulation of the incremental and the "affine" methods or the "isotropic" approximation which delivers better results at the overall scale.

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Thermomechanical behaviour of shape memory alloy

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In copper-based SMAs, it has been experimentally shown that, below their martensite start temperature Ms, the material microstructure is constituted of twenty-four active variants embedded into six self-accommodated groups; each group is composed of four variants. Under no applied stress, all these variants have equal probability of growing; but loading the material transforms the polyvariant microstructure into an homogenous one formed by the most favourably oriented variant with respect to the loading conditions . To take into account this microstructure evolution involved by the reorientation strain mechanism ,we present, in this work the element of the thermomechanical behaviour of single and polycrystal in transformation plasticity using Taylor's approach. The problem is studied by mean of kinematics analysis and thermodynamic approach. We also put out the contribution of the variant's reorientation mechanism to the micromechanical behaviour. These results give us useful indication for optimal use of SMAs in applications .

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Multiscale Dislocation Dynamics Plasticity

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A framework for investigating size-dependent small-scale plasticity phenomena and related material instabilities at various length scales ranging from the nano-microscale to the mesoscale is presented. The model is based on fundamental physical laws that govern dislocation motion and their interaction with various defects and interfaces. Particularly, a multi-scale model is developed merging two scales, the nano-microscale where plasticity is determined by explicit three-dimensional dislocation dynamics analysis providing the material length-scale, and the continuum scale where energy transport is based on basic continuum mechanics laws. The result is a hybrid simulation model coupling discrete dislocation dynamics with finite element analyses. With this hybrid approach, one can address complex size-dependent problems, including dislocation boundaries, dislocations in heterogeneous structures, dislocation interaction with interfaces and associated shape changes and lattice rotations, as well as deformation in nano-structured materials, localized deformation and shear bands.

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PREDICTION OF MECHANICAL PROPERTIES AND DAMAGE EVOLUTION IN POLYMERIC COMPOSITES THROUGH MESO-MECHANICAL MODELLING

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A class of materials which are gaining ever increasing industrial applications are polymers and polymer composites. A sub-class is epoxy polymers and fibre-reinforced epoxy composites. Epoxy resins are crosslinked polymers and *partially* crystalline. Because of complexity of the spatial arrangement of molecular chains of polymer and disorders contained therein, the constitutive modeling of polymers has been mostly based on a rheological and/or phenomenological formulation.

In the case of fibre-reinforced polymeric composites, a structure composed of unit cells can be defined which could represent the periodic nature of the material. The scale of cells in this structure is of the order of the fiber diameter, generally in μm. A further higher scale can be constructed by homogenization of fibres into strands embed in the matrix in a meso-scale (of the order of 100 μm). In this paper a three-dimensional multi-cell representative volume element is analyzed by finite element method. The analysis predicts the stress/strain field at the fibre and matrix, at the interfaces between the fibre and matrix and between the layers, as well as the over all (macroscopic) mechanical behaviour.

Furthermore, the evolution of damage initiation and propagation in cross-ply laminates is studied. This meso- mechanical representation is based on the known properties of the constituents (fibre and matrix) and the assumption that the composite material possesses a periodic structure. The epoxy matrix is represented by a nonlinear viscoelastic constitutive model whereas the fibre is assumed to remain elastic.

In this presentation, the effect of viscoelastic matrix and the resulting time-dependent behaviour on the evolution of residual stresses arising from the manufacturing process, and damage initiation and propagation due to externally applied loads, will be presented.

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RESPONSE OF Ti-6Al-4V ALLOYS OVER A WIDE RANGE OF STRAIN RATES AND TEMPERATURES, AND CONSTIUTUTIVE MODELING

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A comprehensive study of the response of Ti-6Al-4V alloys, subjected to quasi-static and dynamic loads, will be described. Experiments on these alloys were conducted over a wide strain-rate range of 10 E-6 to 10E+3 per second, and at temperatures ranging from –100 to 900 F. Strain rate jump experiments and uniaxial to biaxial compression experiments were also perfoprmed. The correlations between Johnson-Cook (J-C) and Khan-Huang-Liang (KHL) models, and experimental results at constant strain rate tests were made after determining material constants from the same experimental data. It is shown that KHL model correlates better than J-C model with the observations. Using these material constants, predictions from the two models are made for the strain-rate jump and uniaxial to biaxial compression experiments.The predictions from KHL model are definitely closer to the experimental results than J-C model.

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A Stress-Strain Mixture Law Without Fitting Parameter. Application to Several Classical Problems of Heterogeneous Material Behaviour.

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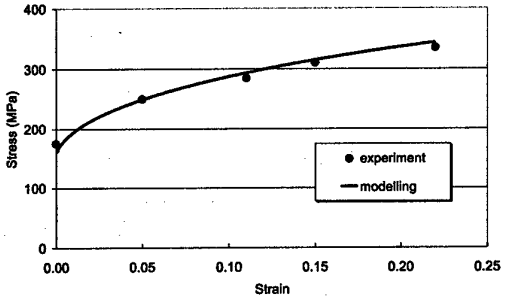
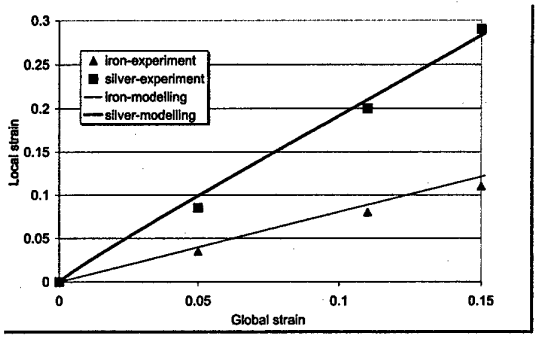
Assuming an equi-incremental mechanical work in each constituent in stress-strain mixture law (i.e $\sigma_1 \cdot d\varepsilon_1 = \sigma_2 \cdot d\varepsilon_2$), this article focuses on the interest of this approach trough comparison with others modelling methods as Taylor, Sachs self-consistent or finite element modelling. In a first part, the study shows how this assumption avoid any arbitrary fitting parameter in mixture law on the contrary of classical variants. In a second part, miscellaneous applications are illustrated for some heterogeneous materials mechanical behaviour problems as two constituent elasticity and plasticity or two dislocation densities composite type model. This approach has shown :
a more realistic description than simple mixture rule on stress,
a non necessity of any arbitrary fitting parameter for intermediate mixture rule on stress and strain,
a respect of theoretical bounds of homogeneization methods,
an accuracy close to heavier method as self-consistent modelling but so far more simple to use.
In conclusion this modelling (IsoW) seems to improve the ratio between accuracy and sophistication of heterogeneous material behaviour modelling.



a. flow stres



b. local strains

Figure : Example of IsoW modelling results for a composite Fe-Ag18%

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On anisotropic formulations of multiplicative inelasticity

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The paper will address two issues. First the formulation of an anisotropic law for the thermodynamical stress, and second, the inclusion of kinematical hardening effects in the formulation of the free energy function.

A possible anisotropy of the constitutive law for the stress tensor plays a dominant role within multiplicative theories of inelasticity. On the theoretical side, it decides about the form of the reduced dissipation inequality, and hence about the formulation of some evolution equations which have to stand in accord with the mentioned inequality. On the numerical side, it dictates to a wide extend the solution schemes to be adopted in a numerical analysis. The paper aims at a study of the implications with regard to such an anisotropy. That is, we study the implications of the formulation of an anisotropic free energy function. In so doing we rely on a structural tensor-based description, where the free energy is understood as an isotropic function of specific agencies consisting of an adequately defined elastic strain tensor and a set of adequately defined structural tensors which specify the kind of anisotropy under consideration.

Different formulations are provided depending on the homogenization procedures adopted. In addition, the volumetric isochoric split, well known and intensively applied in finite strain isotropic formulations, is discussed and its possible applicability to the anisotropic case is illuminated.

Further anisotropic effects are provided by the inclusion of the back stress in the formulation to describe the so called kinematical hardening. The extension of small strain formulations to the large strain case is, in the presence of the back stress, by no means trivial and necessitates a special discussion. In the large strain case, and with an eye on anisotropy, the theoretical development is naturally carried out in a material frame. Evolution equations in term of material time derivatives result, anyhow, in back stress tensors which are not symmetric once pushed-forward to the actual configuration; a fact with no experimental evidence. Alternatively, the inclusion of kinematical hardening effects can be considered in the definition of the free energy function. Here too, the symmetry of the back stress is an issue and will be addressed. It is shown that a certain geometrical structure must be preserved in order for the mentioned symmetry not to be violated.

All cases are illustrated using numerical examples of inelastic deformations at finite strains. Specifically, evolution equations of the unified type are used.

DEEP DRAWING PROCESS OF AN AISI304 STAINLESS STEEL : INTERACTION BETWEEN GEOMETRY TOOLS AND KINETICS OF PLASTIC INDUCED MARTENSITE FROM A MICROMECHANICAL FRAMEWORK

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Mechanisms of transformation plasticity deformation are reviewed for martensitic transformation of stainless steel material. It is well established that the origin of transformation plasticity is especially attributed to the orientation of the plastic yielding around the transforming particles when deformations are plastically accommodated. This mechanism is also related to the applied stress, the mechanical properties of each phase and the progress of the transformation. On the other hand, the transformation strains may be accommodated elastically, plastically or by self accommodation. For martensitic transformation, two components of transformation can be distinguished: a volume variation which can be accommodated elastically and/or plastically, and a shear strain. The shear strain accommodation can be realized by twinning, slip in martensite or in austenite. For martensitic transformation, accommodation for transformation strains may be modified when transformation occurs during cooling or during tensile test for example. Moreover, depending on the stress state, these accommodation processes can be modified if the material is subjected to a large plastic deformation. In this case, accommodation by slip in austenite may be favoured. The main purpose of the present work consists in the analysing of the interaction between the kinetic of the martensitic transformation in the AISI304 stainless steel from a micromechanical viewpoint, and the geometric parameters in the deep drawing process (die profile radius, punch radius,...) and the boundary conditions (Blank holding force, friction, ...). We try to elucidate, basing on a good description of the hardening behaviour, that the optimisation of the tool geometry in drawing process, are quite important to obtain better predictions of load levels and strain distribution of the metastable stainless steel. These improvements are illustrated by numerical calculations performed with our new hardening and yield models.

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Modeling and simulation of dynamic plasticity and failure in ductile metals

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The optimisation of the manufacturing process involving high strain rates or the description of classical impact tests require a deep understanding of the material behavior. The Mechanical Threshold Stress model (MTS), developed by Follansbee and Kocks, is shown to be of great interest to capture the material response for a large range of strain rates and temperature. To perform a complete numerical simulation of high strain rate processes such as blanking and Taylor impact test, the MTS model is implemented in the finite element code ABAQUS/Explicit and combined with a Nucleation And Growth (NAG) approach for damage. Both the MTS and The NAG model are based on dislocation motion theory. Here the damage variable, denoted d, which is linked to the material porosity by a self consistent approach affects the elastic constants as well as the hardening rate, denoted θ. This variable is given by :

$$d = \frac{15(1-\upsilon)}{(7-5\upsilon)} f_v$$

where f_v is the porosity in the material and ν is the Poisson ratio.
The effect of damage on the hardening rate is expressed by introducing a damage function D, which characterizes the ductility of the material, in the classical expression of the hardening rate as follows :

$$\theta = D\left(\frac{d_c - d}{d_c}\right)\theta_{MTS} \quad \theta_{MTS} = \theta_0\left(1 - F\left(\frac{\hat{\sigma} - \hat{\sigma}_a}{\hat{\sigma}_S - \hat{\sigma}_a}\right)\right)$$

where θ_{MTS} is the hardening rate of the non damaged material given by Follansbee and Kocks and F is a function, which depends on the considered material, of the thermal component of the mechanical threshold stress $\hat{\sigma}$.The term $\hat{\sigma}_a$ is the athermal component of the MTS model that is rate independent, $\hat{\sigma}_s$ the saturation stress and d_c is the critical value of damage.

We simulate the Taylor impact test, the planar impact test and high stroke rate blanking process with our model. Copper is the considered material for these tests. We discuss our results in comparison with those of the Johnson-Cook model for these tests. The simulated results from both models are also compared with the experimental ones.

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Effects of polymeric additives on the morphology and the structure of the calcium carbonate material

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In this work, we investigate the crystallisation of calcium carbonate (CaCO3) from supersaturated solutions and in the presence of polymeric additives. Depending on the nature and concentration of the additive used, we obtain various calcium carbonate particles having different sizes, crystalline structures and morphologies. Thus, with pure non-ionic copolymers, the mineral crystallisation gives birth to CaCO3 agglomerate of primary particles with a size of few microns, which present mostly rhombohedral morphologies. On the other hand, in the presence of the pure anionic polyelectrolyte, we obtain CaCO3 crystals having smooth spherical shape. Further, in the presence of additive made of copolymer-polyelectrolyte mixture, the calcium carbonate crystallisation gives birth to modified CaCO3 crystals morphologies. Such morphologies are function of the ratio I, $I=C_{copolymer}/C_{polyelectrolyte}$, where $C_{copolymer}$ and $C_{polyelectrolyte}$, are respectively, the copolymer and the polyelectrolyte concentrations used. Hence, at low I values, the calcium carbonate crystallization gives rough CaCO3 spherical, while at high I values, we observe elongated CaCO3 particles.

The CaCO3 crystal structures obtained by the X-ray analyses were pure calcite when the additive is the non-ionic copolymer and pure vaterite in the presence of the anionic polyelectrolyte. The data obtained indicate that the pure polyelectrolyte inhibits the crystal growth in all directions and lead to homogenous CaCO3 spherical particles. However in the presence of the copolymer-polyelectrolyte mixture, the crystal growth seems to be inhibited in preferential directions.

This study shows that the morphology and structure of the CaCO3 crystals can be controlled by the use of either pure or mixture polymers. Finally, the effects of the polyelectrolyte and non-ionic copolymer on the precipitation of the CaCO3 are explained in terms of two main mechanisms involving ion exchange and/or ion complexation and preferential adsorption.